



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:38 PM UTC

PDB ID : 6UTQ / pdb_00006utq
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

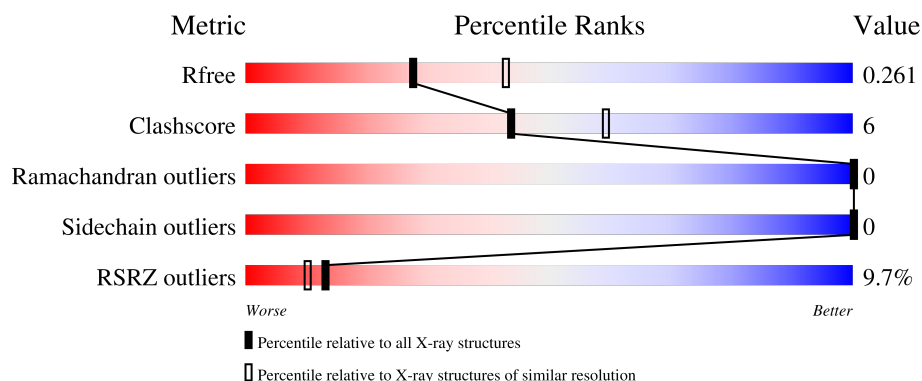
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	13% 72% 14% 14%
1	B	286	3% 76% 9% 14%
1	C	286	3% 76% 11% 13%
1	D	286	7% 73% 10% 16%
1	E	286	20% 67% 17% 16%

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Mol	Chain	Length	Quality of chain
1	F	286	

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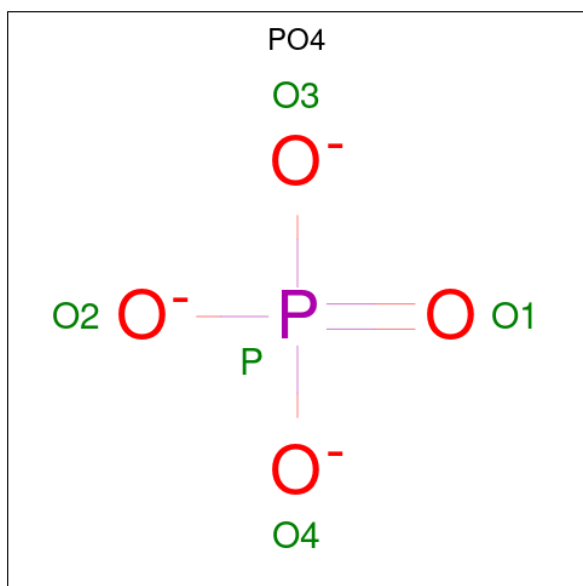
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Chain	Residue	Modelled	Actual	Comment	Reference
F	286	LYS	-	expression tag	UNP A0A0G9FES3

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



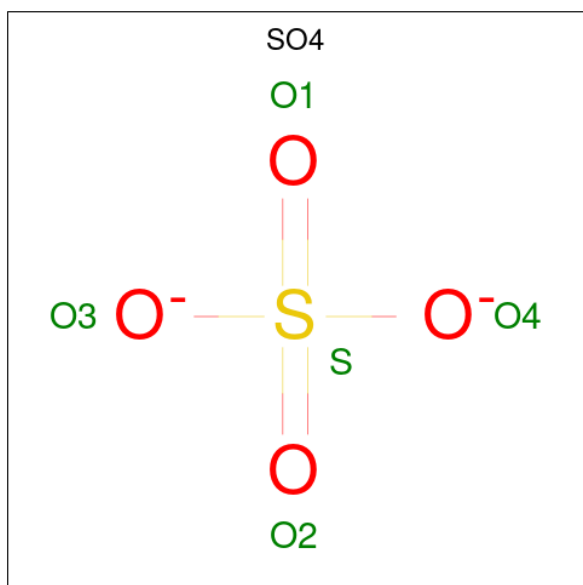
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

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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 (CCD ID: SO4) (formula: O₄S).



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		

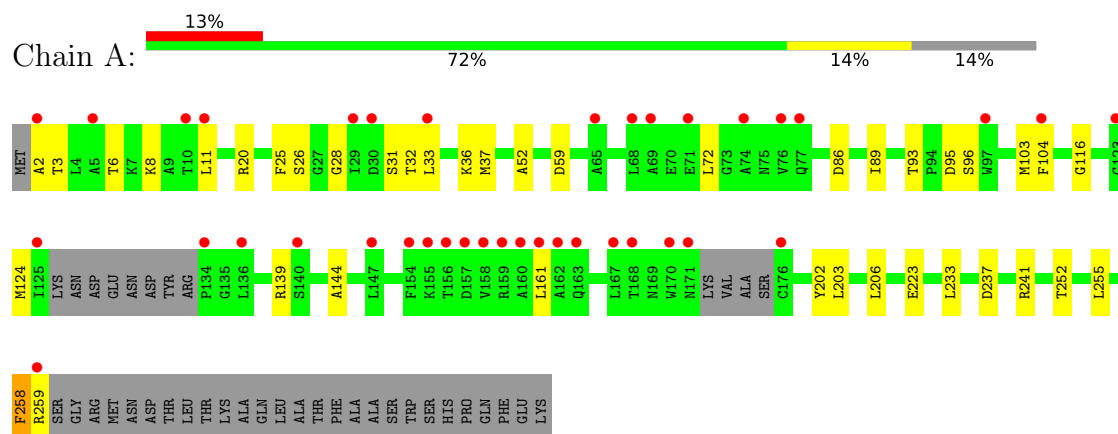
- Molecule 5 is water.

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

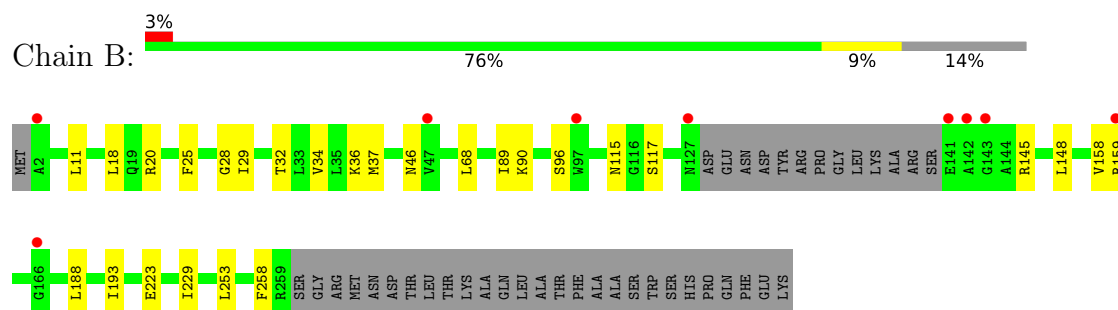
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

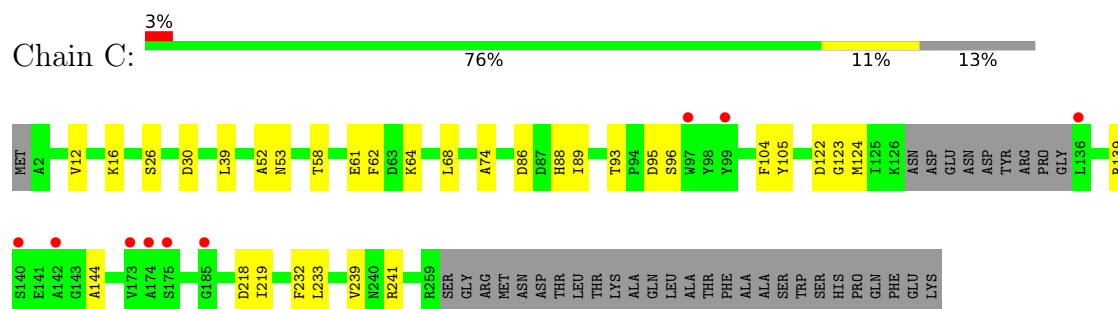
- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



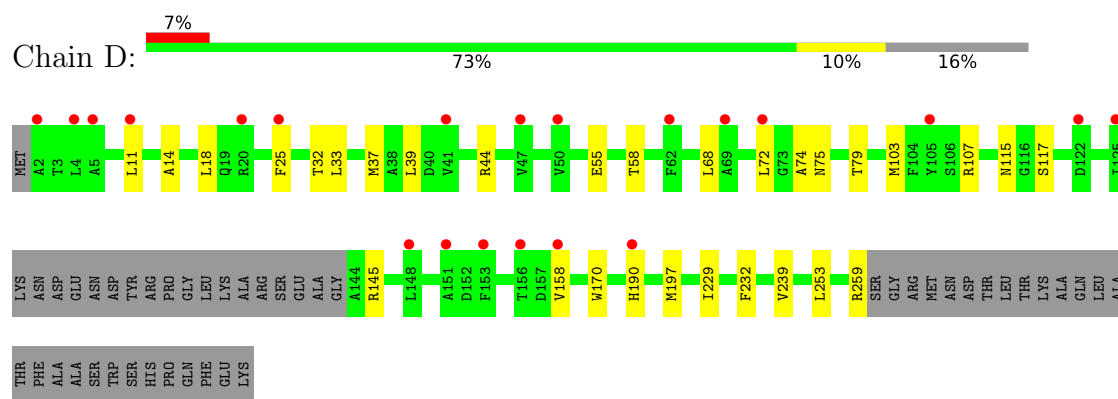
- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



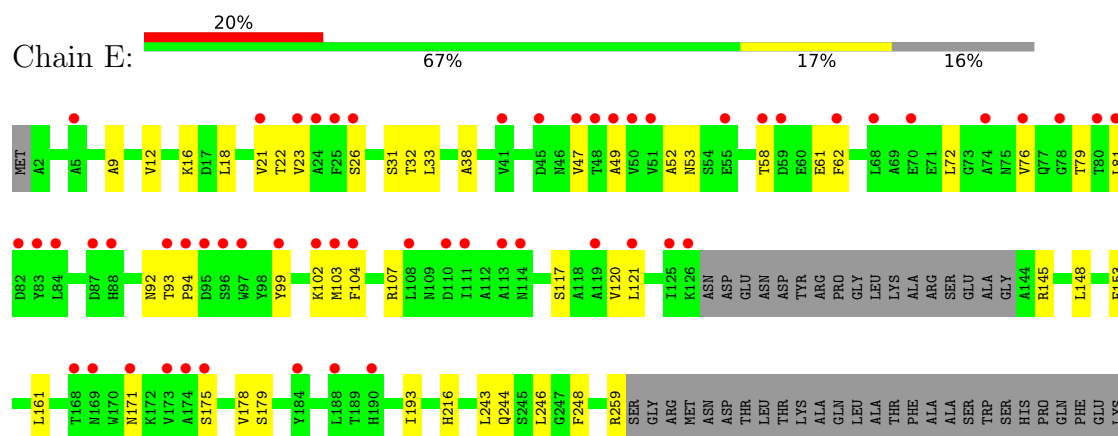
- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



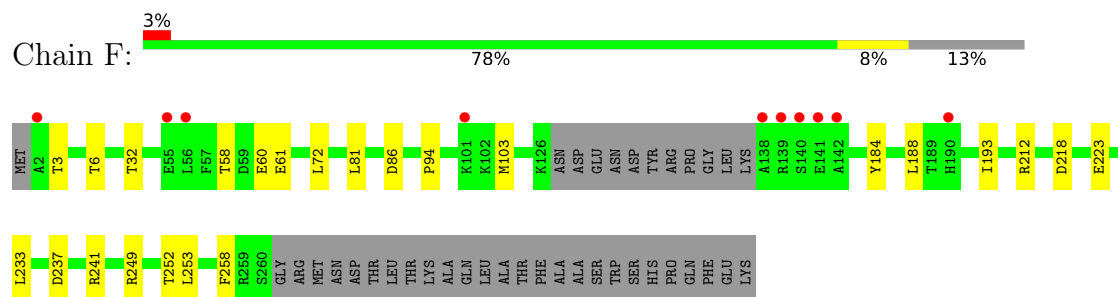
- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



• 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, α , β , γ	107.78Å 107.78Å 319.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.88 – 2.39 37.88 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.88-2.39) 99.3 (37.88-2.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, R_{free}	0.213 , 0.254 0.222 , 0.261	Depositor DCC
R_{free} test set	3790 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CD, PO4, 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	0.49	1/1891 (0.1%)	0.72	1/2566 (0.0%)
1	B	0.39	0/1897	0.63	2/2574 (0.1%)
1	C	0.40	0/1928	0.59	0/2614
1	D	0.43	0/1855	0.63	0/2519
1	E	0.42	0/1795	0.68	0/2443
1	F	0.38	0/1916	0.59	0/2597
All	All	0.42	1/11282 (0.0%)	0.64	3/15313 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	PHE	C-N	-7.67	1.22	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	PHE	O-C-N	6.79	131.03	123.01
1	B	158	VAL	CA-C-N	-6.69	111.51	122.54
1	B	158	VAL	C-N-CA	-6.69	111.51	122.54

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	29	0
1	B	1868	0	1824	19	0
1	C	1899	0	1868	20	0
1	D	1826	0	1763	20	0
1	E	1767	0	1673	32	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	134	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 (134) 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:C:93:THR:OG1	1:C:95:ASP:OD1	2.08	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:11:LEU:HG	1:A:37:MET:HE2	1.79	0.63
1:D:39:LEU:HD11	1:D:74:ALA:HB2	1.81	0.62
1:F:86:ASP:HB2	1:F:103:MET:HE1	1.81	0.61
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:A:233:LEU:HD11	1:F:233:LEU:HD11	1.91	0.52
1:E:93:THR:HG22	1:E:94:PRO:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ASN:OD1	1:B:117:SER:OG	2.23	0.51
1:D:79:THR:HG1	1:D:107:ARG:HH11	1.58	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
1:D:145:ARG:HH11	1:D:145:ARG:HG3	1.76	0.50
1:A:86:ASP:HB2	1:A:103:MET:HE1	1.94	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: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: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:58:THR:HG22	1:D:197:MET:HE2	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:A:124:MET:HE3	1:A:139:ARG:HD3	1.97	0.46
1:A:8:LYS:HD2	1:A:8:LYS:C	2.41	0.46
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:OD1	1:F:218:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:MET:HE2	1:C:139:ARG:HD3	2.00	0.44
1:C:219:ILE:HD11	1:E:216:HIS:ND1	2.32	0.44
1:C:105:TYR:OH	1:C:122:ASP:OD2	2.33	0.44
1:E:31:SER:OG	4:E:302:SO4:O1	2.35	0.44
1:A:20:ARG:HH21	1:A:116:GLY:C	2.26	0.44
1:A:255:LEU:HD21	1:F:253:LEU:HB2	2.00	0.44
1:D:103:MET:HE2	1:D:103:MET:HB3	1.74	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
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:81:LEU:HA	1:F:81:LEU:HD23	1.77	0.42
1:F:94:PRO:HA	1:F:184:TYR:CE1	2.54	0.42
1:D:11:LEU:HD23	1:D:37:MET:HE2	2.00	0.42
1:D:145:ARG:HG3	1:D:145:ARG:NH1	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: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:HD23	1:A:203:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:MET:HE3	1:E:103:MET:HB2	1.75	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 [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	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 [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	189/236 (80%)	189 (100%)	0	100	100
1	B	192/236 (81%)	192 (100%)	0	100	100
1	C	196/236 (83%)	196 (100%)	0	100	100
1	D	186/236 (79%)	186 (100%)	0	100	100
1	E	169/236 (72%)	169 (100%)	0	100	100
1	F	194/236 (82%)	194 (100%)	0	100	100
All	All	1126/1416 (80%)	1126 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	149	GLN
1	B	171	ASN
1	D	88	HIS
1	D	163	GLN
1	E	88	HIS
1	E	92	ASN
1	E	236	ASN
1	F	163	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	305	-	4,4,4	0.30	0	6,6,6	0.41	0
3	PO4	F	301	-	4,4,4	1.00	0	6,6,6	1.00	0
3	PO4	C	302	-	4,4,4	1.13	0	6,6,6	0.75	0
4	SO4	F	302	-	4,4,4	0.26	0	6,6,6	0.58	0
3	PO4	B	303	-	4,4,4	1.10	0	6,6,6	0.56	0
3	PO4	E	301	-	4,4,4	1.01	0	6,6,6	0.37	0
4	SO4	B	304	-	4,4,4	0.24	0	6,6,6	0.46	0
3	PO4	A	303	-	4,4,4	1.01	0	6,6,6	0.85	0
3	PO4	D	303	-	4,4,4	1.30	0	6,6,6	0.45	0
4	SO4	A	304	-	4,4,4	0.27	0	6,6,6	0.26	0
4	SO4	C	303	-	4,4,4	0.18	0	6,6,6	0.23	0
4	SO4	E	302	-	4,4,4	0.31	0	6,6,6	0.15	0
4	SO4	D	304	-	4,4,4	0.28	0	6,6,6	0.35	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	A	305	SO4	2	0
3	E	301	PO4	1	0
3	D	303	PO4	2	0
4	C	303	SO4	1	0
4	E	302	SO4	2	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, 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	246/286 (86%)	0.93	38 (15%) 5 4	48, 71, 98, 109	0
1	B	245/286 (85%)	0.39	9 (3%) 45 41	41, 59, 81, 96	0
1	C	249/286 (87%)	0.40	9 (3%) 46 42	43, 60, 81, 98	0
1	D	240/286 (83%)	0.82	21 (8%) 15 12	46, 69, 90, 97	0
1	E	241/286 (84%)	1.27	56 (23%) 2 1	49, 92, 116, 121	0
1	F	248/286 (86%)	0.37	10 (4%) 42 38	48, 59, 79, 110	0
All	All	1469/1716 (85%)	0.69	143 (9%) 13 10	41, 64, 103, 121	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	140	SER	5.2
1	A	156	THR	5.0
1	A	171	ASN	4.8
1	C	185	GLY	4.5
1	B	142	ALA	4.4
1	E	173	VAL	4.2
1	F	141	GLU	4.2
1	B	143	GLY	4.1
1	C	136	LEU	4.0
1	C	97	TRP	4.0
1	A	170	TRP	3.9
1	E	47	VAL	3.8
1	F	2	ALA	3.8
1	E	110	ASP	3.7
1	E	80	THR	3.7
1	E	87	ASP	3.7
1	A	134	PRO	3.7
1	E	49	ALA	3.6
1	F	138	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	4	LEU	3.6
1	A	29	ILE	3.5
1	E	174	ALA	3.5
1	B	127	ASN	3.5
1	A	136	LEU	3.4
1	A	2	ALA	3.4
1	E	171	ASN	3.3
1	E	45	ASP	3.3
1	E	88	HIS	3.3
1	E	50	VAL	3.3
1	D	125	ILE	3.2
1	B	166	GLY	3.2
1	A	161	LEU	3.2
1	C	140	SER	3.1
1	E	82	ASP	3.1
1	D	2	ALA	3.1
1	D	41	VAL	3.1
1	E	95	ASP	3.1
1	A	5	ALA	3.1
1	A	97	TRP	3.0
1	A	157	ASP	3.0
1	A	259	ARG	3.0
1	F	142	ALA	3.0
1	E	23	VAL	3.0
1	E	76	VAL	3.0
1	F	190	HIS	3.0
1	E	97	TRP	3.0
1	E	108	LEU	2.9
1	A	68	LEU	2.9
1	E	84	LEU	2.9
1	D	156	THR	2.9
1	A	69	ALA	2.9
1	A	167	LEU	2.9
1	E	104	PHE	2.9
1	E	119	ALA	2.9
1	F	139	ARG	2.9
1	A	159	ARG	2.9
1	E	102	LYS	2.8
1	B	2	ALA	2.8
1	E	62	PHE	2.8
1	E	111	ILE	2.8
1	E	24	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	41	VAL	2.8
1	D	105	TYR	2.7
1	C	173	VAL	2.7
1	A	71	GLU	2.7
1	A	10	THR	2.7
1	F	101	LYS	2.7
1	E	113	ALA	2.7
1	D	158	VAL	2.7
1	E	51	VAL	2.7
1	E	58	THR	2.7
1	A	162	ALA	2.6
1	E	96	SER	2.6
1	E	126	LYS	2.6
1	D	25	PHE	2.6
1	D	69	ALA	2.6
1	E	103	MET	2.6
1	E	21	VAL	2.6
1	A	125	ILE	2.6
1	A	140	SER	2.6
1	E	99	TYR	2.6
1	D	190	HIS	2.6
1	E	93	THR	2.5
1	D	47	VAL	2.5
1	B	141	GLU	2.5
1	D	72	LEU	2.5
1	E	175	SER	2.5
1	A	74	ALA	2.5
1	E	114	ASN	2.5
1	E	26	SER	2.5
1	B	47	VAL	2.4
1	B	97	TRP	2.4
1	A	155	LYS	2.4
1	A	168	THR	2.4
1	B	159	ARG	2.4
1	E	70	GLU	2.4
1	E	94	PRO	2.3
1	A	77	GLN	2.3
1	E	81	LEU	2.3
1	D	122	ASP	2.3
1	E	59	ASP	2.3
1	C	99	TYR	2.3
1	E	74	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	30	ASP	2.3
1	C	142	ALA	2.3
1	D	5	ALA	2.3
1	A	176	CYS	2.3
1	A	65	ALA	2.3
1	C	175	SER	2.3
1	E	190	HIS	2.3
1	A	33	LEU	2.2
1	A	158	VAL	2.3
1	E	184	TYR	2.2
1	D	62	PHE	2.2
1	D	153	PHE	2.2
1	A	160	ALA	2.2
1	D	151	ALA	2.2
1	E	125	ILE	2.2
1	A	76	VAL	2.2
1	E	168	THR	2.2
1	E	83	TYR	2.2
1	A	11	LEU	2.2
1	D	148	LEU	2.2
1	E	169	ASN	2.2
1	E	55	GLU	2.2
1	E	78	GLY	2.2
1	E	5	ALA	2.1
1	E	68	LEU	2.1
1	A	154	PHE	2.1
1	A	123	GLY	2.1
1	E	48	THR	2.1
1	A	147	LEU	2.1
1	E	121	LEU	2.1
1	E	188	LEU	2.1
1	A	163	GLN	2.1
1	A	104	PHE	2.1
1	F	55	GLU	2.0
1	D	20	ARG	2.0
1	D	50	VAL	2.0
1	E	25	PHE	2.0
1	C	174	ALA	2.0
1	D	11	LEU	2.0
1	F	56	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

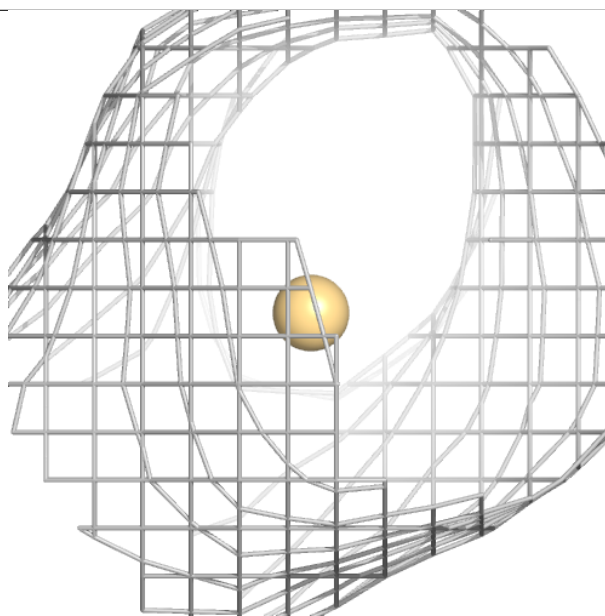
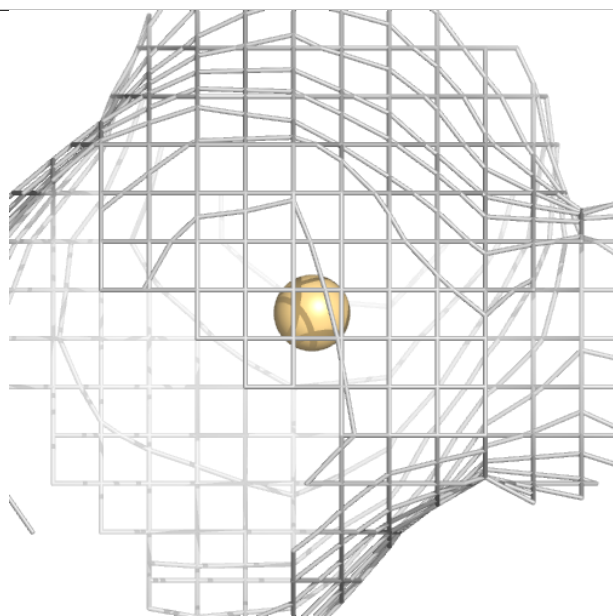
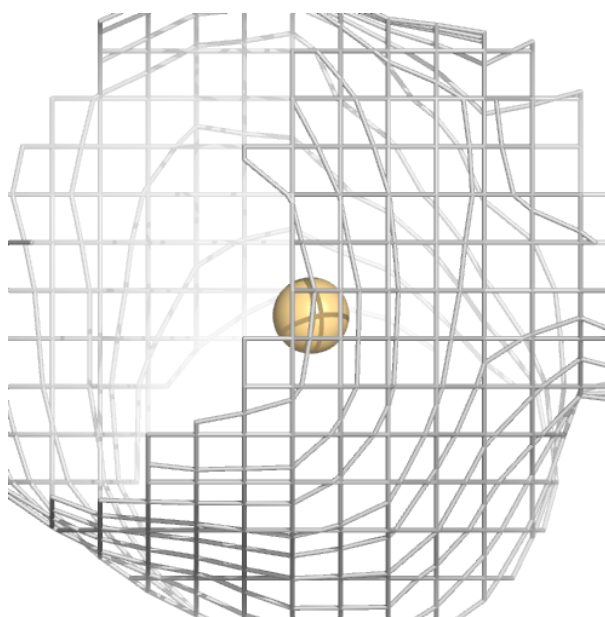
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	305	5/5	0.74	0.16	78,80,81,84	5
4	SO4	D	304	5/5	0.82	0.11	74,83,95,102	0
4	SO4	A	304	5/5	0.89	0.10	69,71,76,80	5
4	SO4	C	303	5/5	0.90	0.09	57,60,68,70	5
4	SO4	F	302	5/5	0.90	0.09	59,63,69,71	0
4	SO4	E	302	5/5	0.91	0.08	79,82,90,90	5
4	SO4	B	304	5/5	0.91	0.10	55,60,64,76	5
3	PO4	F	301	5/5	0.95	0.08	60,61,72,80	0
3	PO4	E	301	5/5	0.96	0.06	70,71,77,88	0
3	PO4	A	303	5/5	0.96	0.07	54,57,64,65	0
3	PO4	C	302	5/5	0.96	0.08	61,62,70,70	0
2	CD	B	301	1/1	0.97	0.06	113,113,113,113	1
2	CD	B	302	1/1	0.97	0.07	78,78,78,78	1
3	PO4	D	303	5/5	0.97	0.06	51,54,65,67	0
2	CD	C	301	1/1	0.97	0.05	118,118,118,118	1
3	PO4	B	303	5/5	0.98	0.05	50,52,53,55	0
2	CD	D	302	1/1	0.98	0.04	114,114,114,114	1
2	CD	A	302	1/1	0.99	0.04	98,98,98,98	1
2	CD	A	301	1/1	0.99	0.03	58,58,58,58	1
2	CD	D	301	1/1	1.00	0.02	61,61,61,61	1

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.

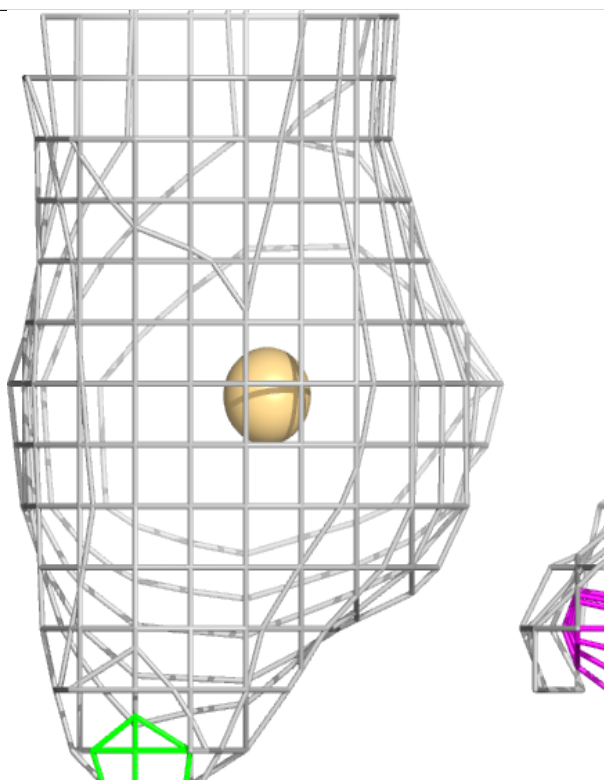
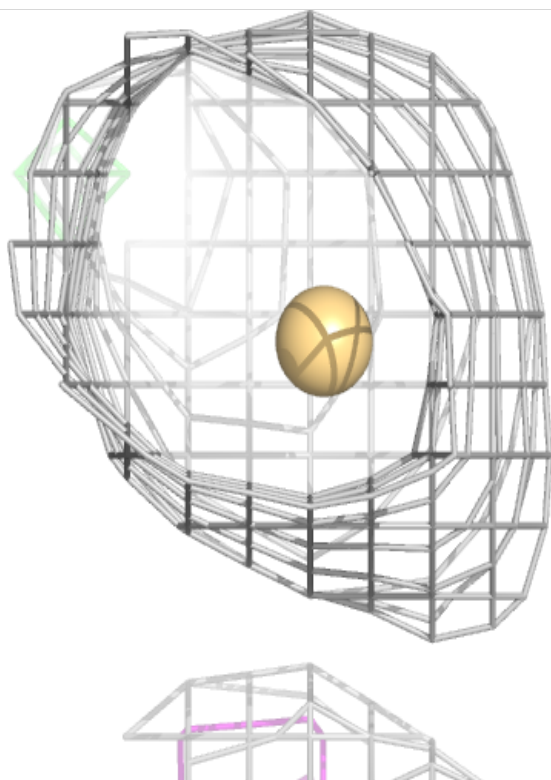
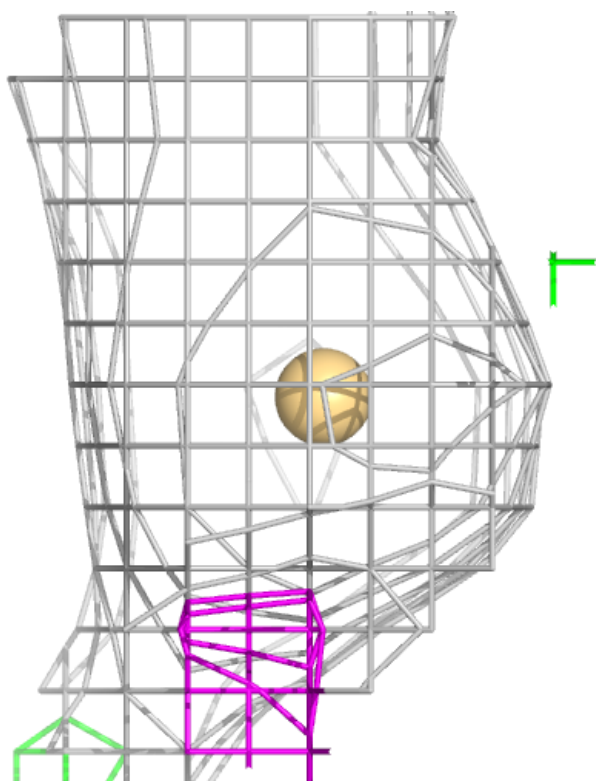
Electron density around CD B 301:

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



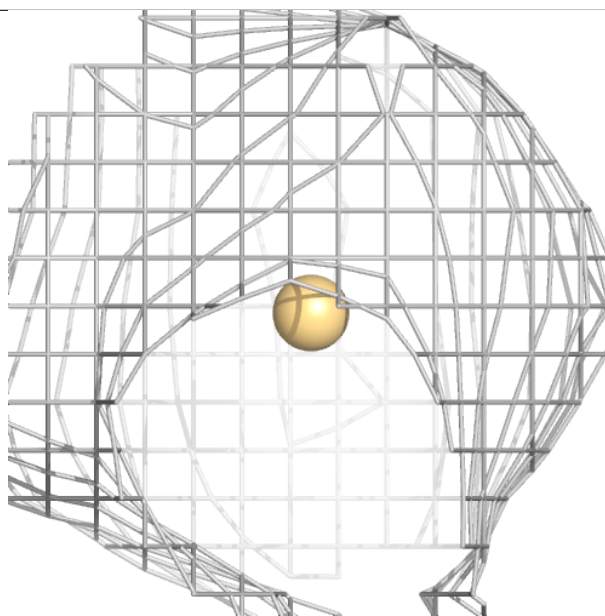
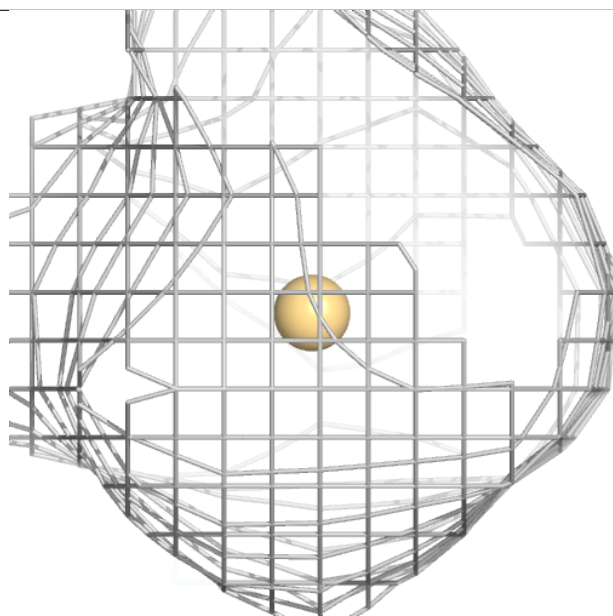
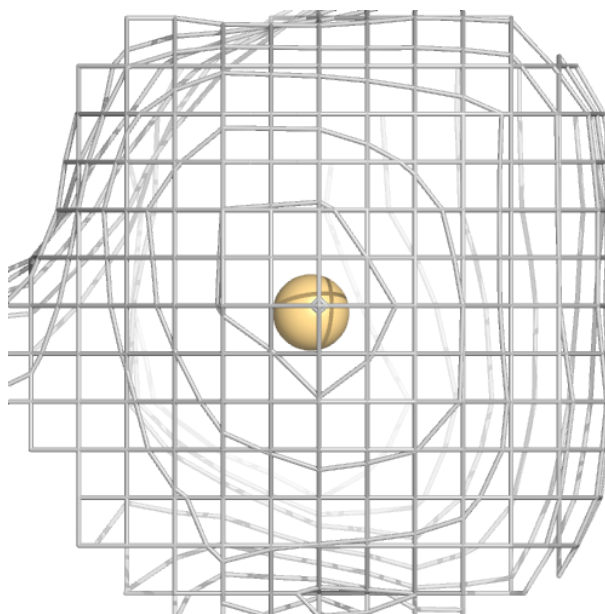
Electron density around CD B 302:

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



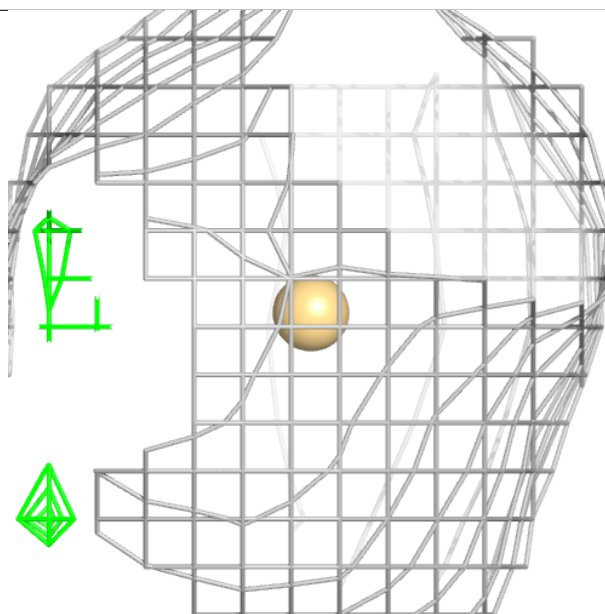
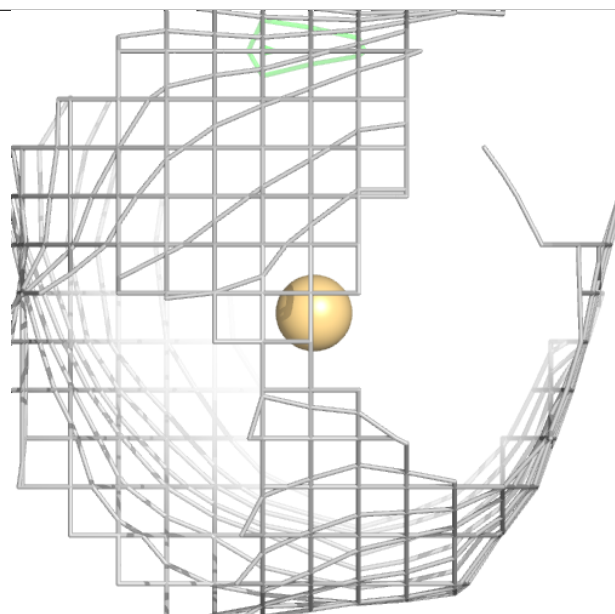
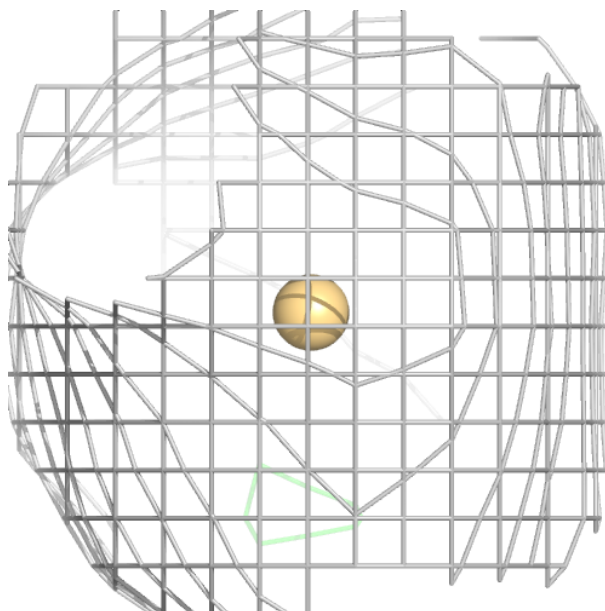
Electron density around CD C 301:

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



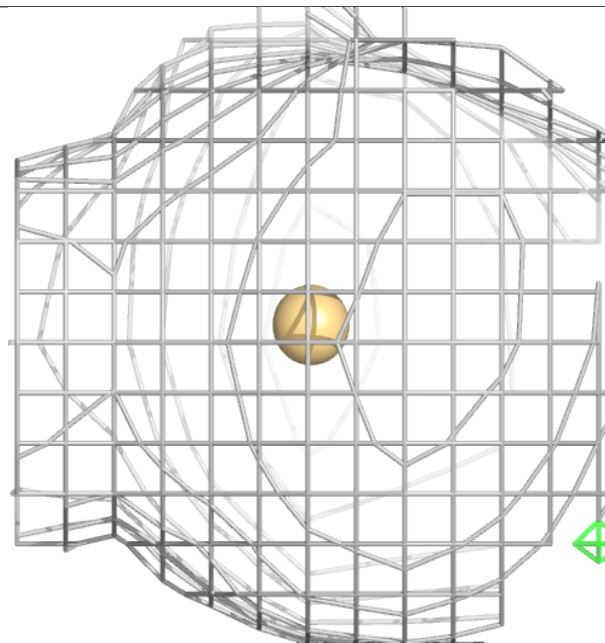
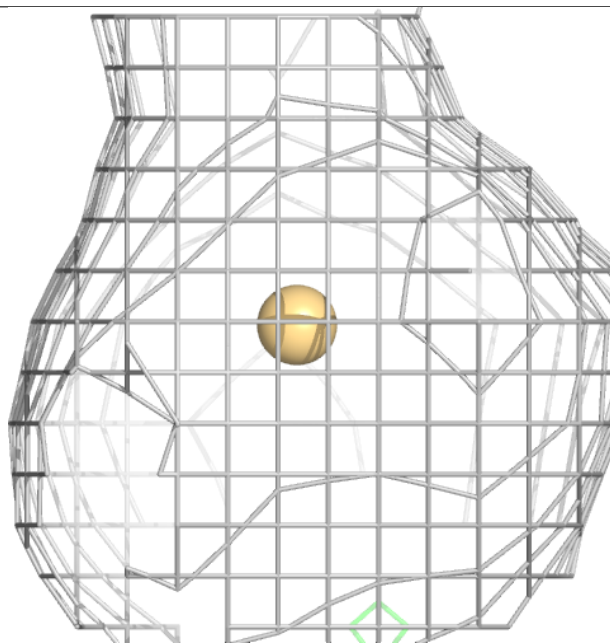
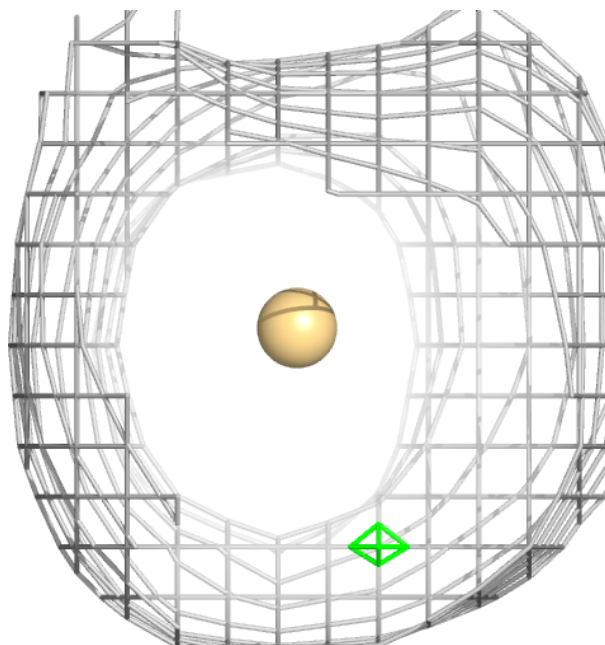
Electron density around CD D 302:

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



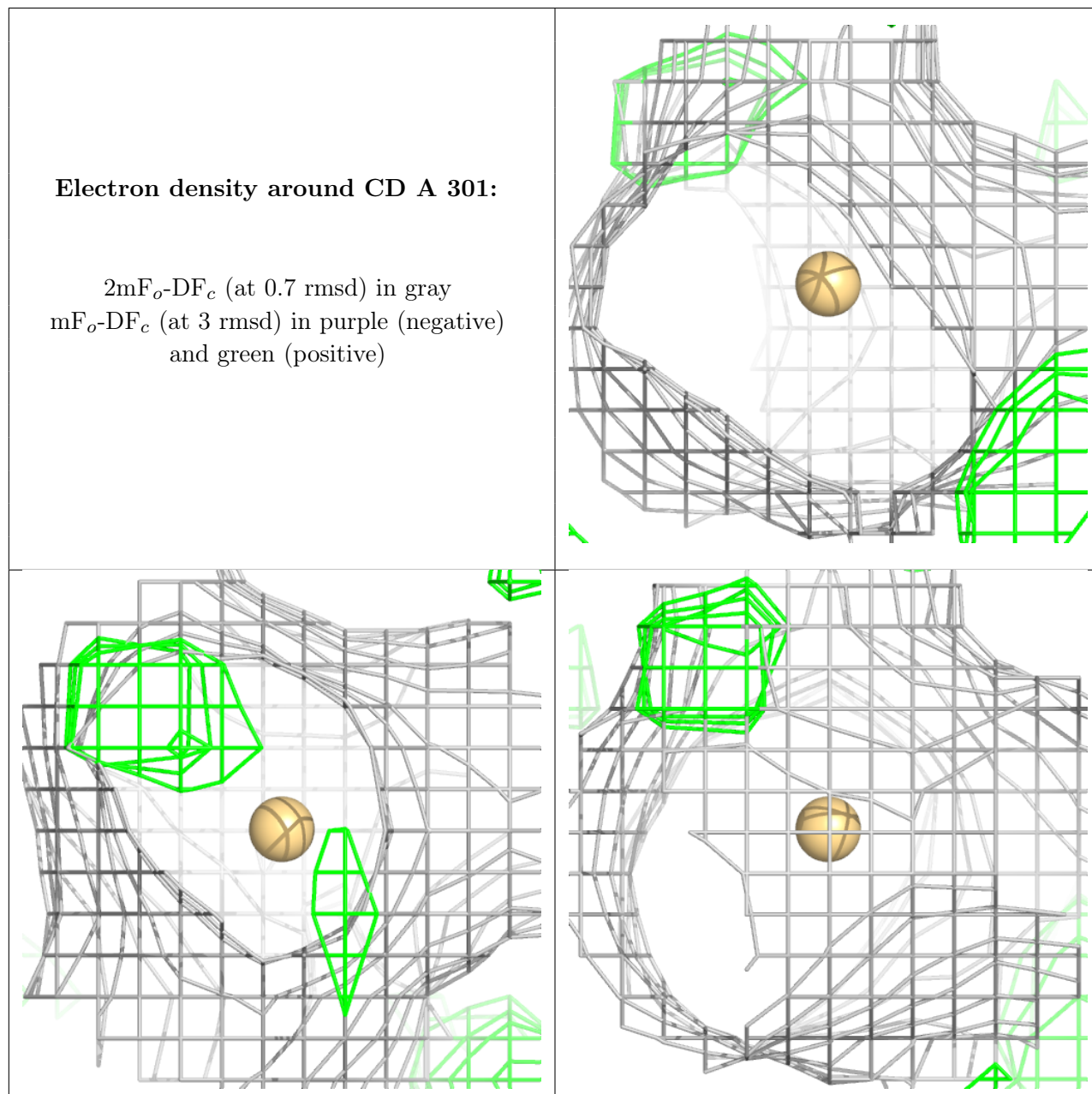
Electron density around CD A 302:

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



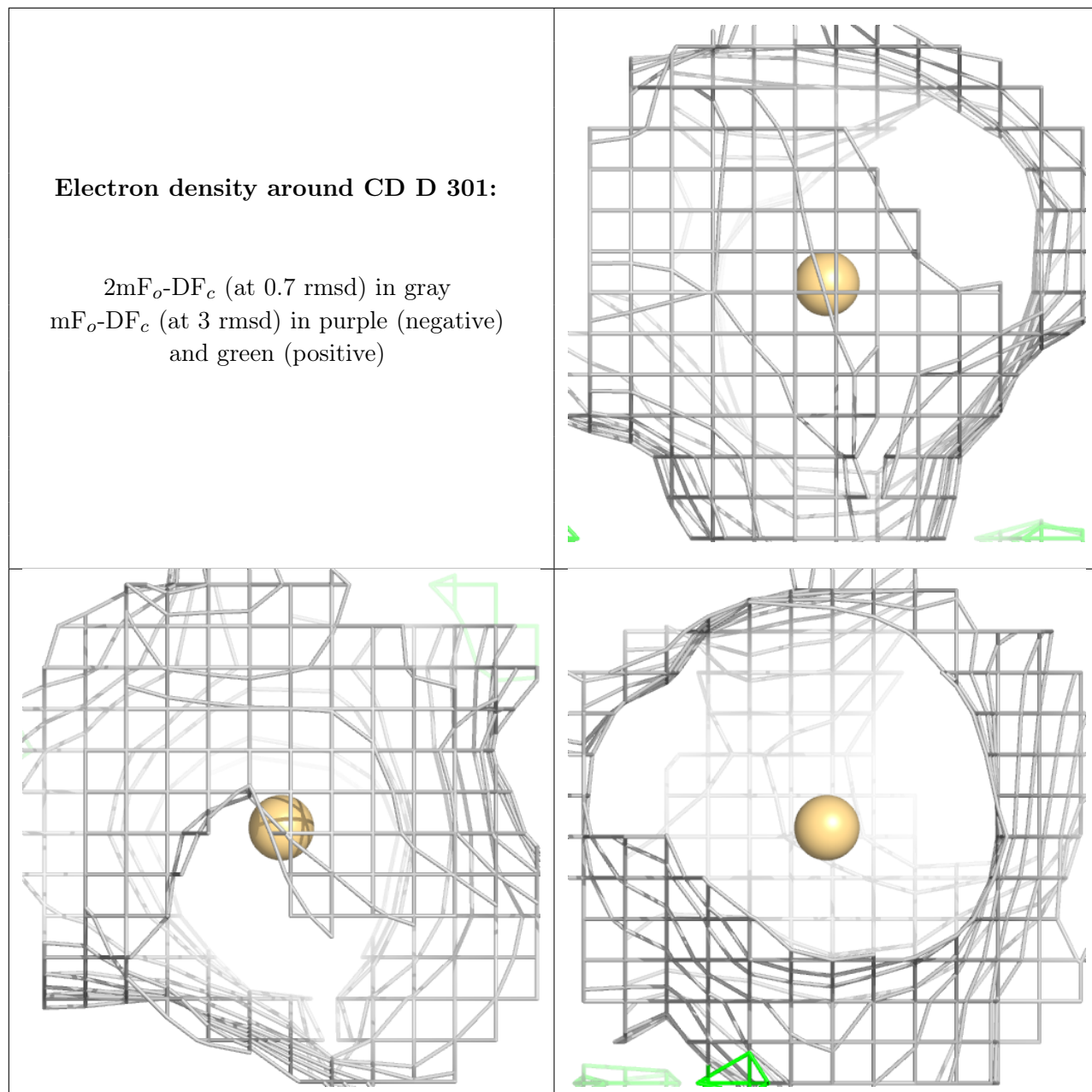
Electron density around CD A 301:

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



Electron density around CD D 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.