



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:25 pm BST

PDB ID : 6UTR
Title : LarE, a sulfur transferase involved in synthesis of the cofactor for lactate racemase in complex with copper
Authors : Fellner, M.; Huizenga, K.; Hausinger, R.P.; Hu, J.
Deposited on : 2019-10-29
Resolution : 2.41 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 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

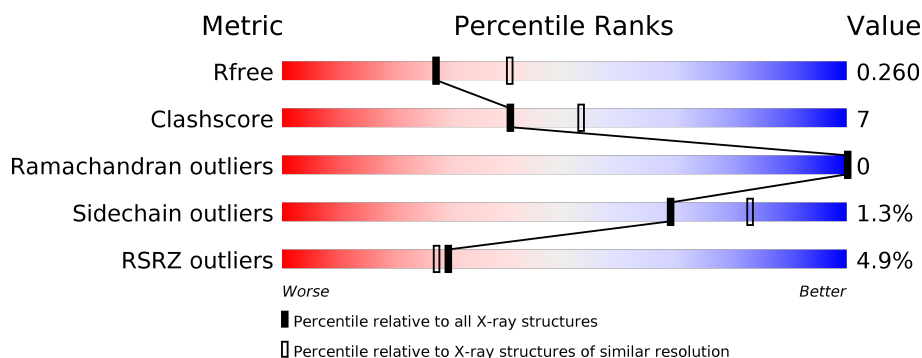
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 ≥ 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>4%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>8%</div> </div> </div>
1	B	286	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>14%</div> </div> </div>
1	C	286	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>13%</div> </div> </div>
1	D	286	<div> <div>9%</div> <div> <div></div> <div>66%</div> <div>15%</div> <div>19%</div> </div> </div>
1	E	286	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>8%</div> </div> </div>
1	F	286	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>14%</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
4	SO4	C	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11580 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	262	Total	C	N	O	S	0	0	0
			1993	1253	348	385	7			
1	B	245	Total	C	N	O	S	0	0	0
			1876	1184	327	359	6			
1	C	249	Total	C	N	O	S	0	0	0
			1919	1210	337	366	6			
1	D	233	Total	C	N	O	S	0	0	0
			1735	1096	303	330	6			
1	E	262	Total	C	N	O	S	0	0	0
			1970	1250	337	376	7			
1	F	247	Total	C	N	O	S	0	0	0
			1908	1200	333	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

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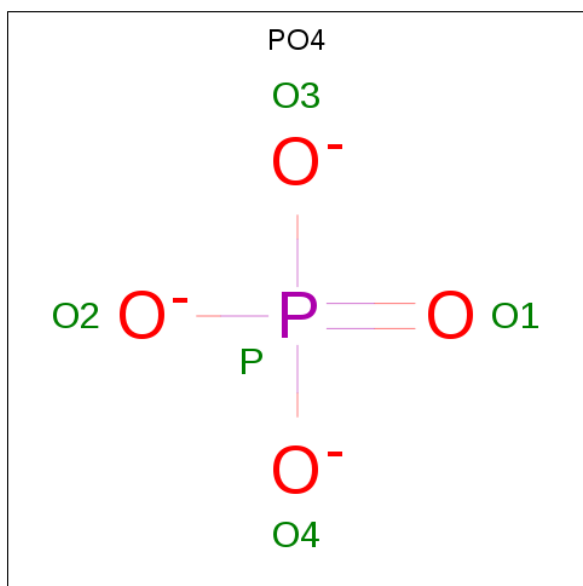
Chain	Residue	Modelled	Actual	Comment	Reference
B	284	PHE	-	expression tag	UNP A0A0G9FES3
B	285	GLU	-	expression tag	UNP A0A0G9FES3
B	286	LYS	-	expression tag	UNP A0A0G9FES3
C	277	ALA	-	expression tag	UNP A0A0G9FES3
C	278	SER	-	expression tag	UNP A0A0G9FES3
C	279	TRP	-	expression tag	UNP A0A0G9FES3
C	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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Chain	Residue	Modelled	Actual	Comment	Reference
F	286	LYS	-	expression tag	UNP A0A0G9FES3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0
3	D	1	Total Cu 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

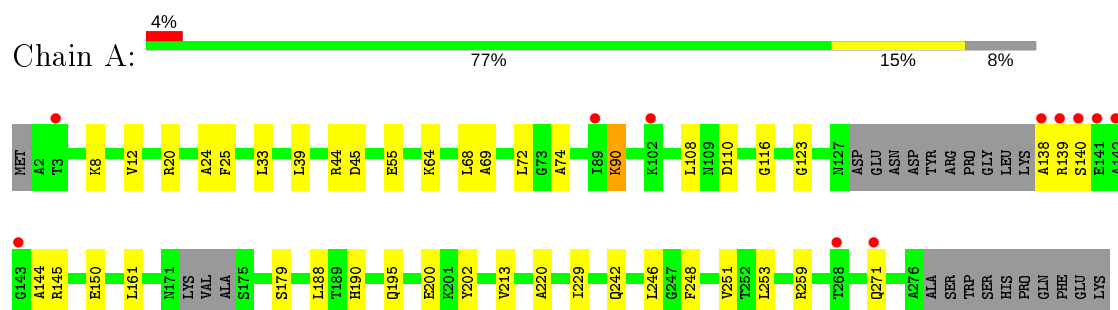
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	26	Total	O	0	0
			26	26		
5	C	16	Total	O	0	0
			16	16		
5	D	13	Total	O	0	0
			13	13		
5	E	21	Total	O	0	0
			21	21		
5	F	22	Total	O	0	0
			22	22		

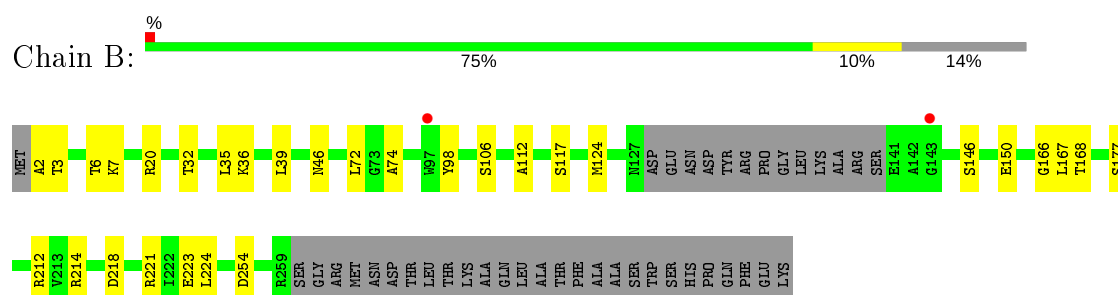
3 Residue-property plots [i](#)

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.

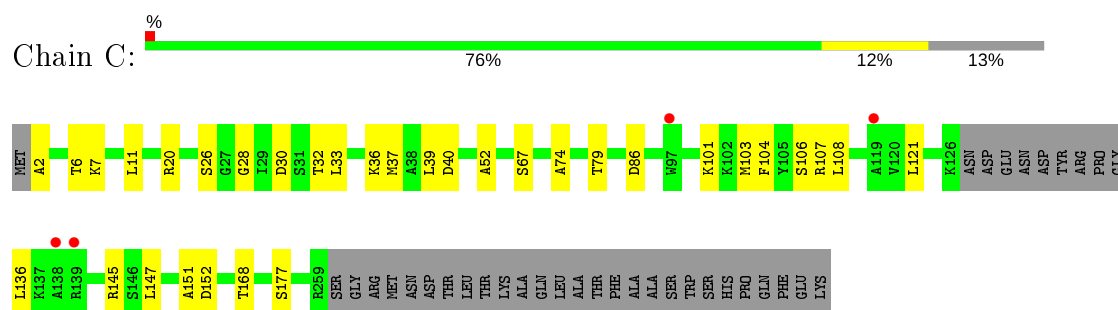
- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

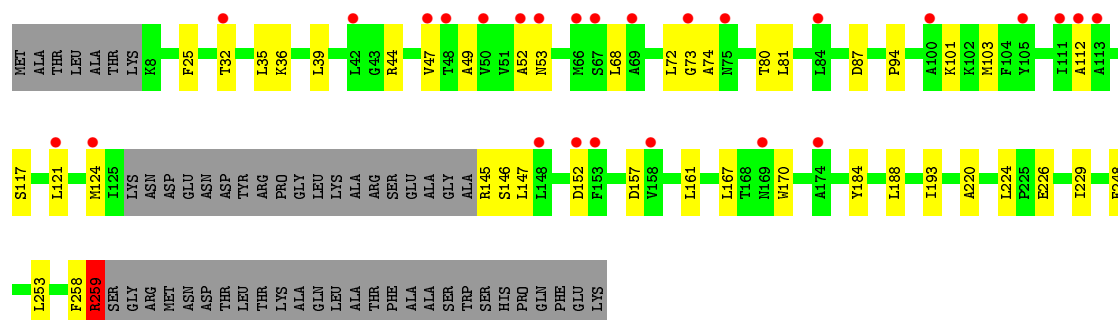


- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

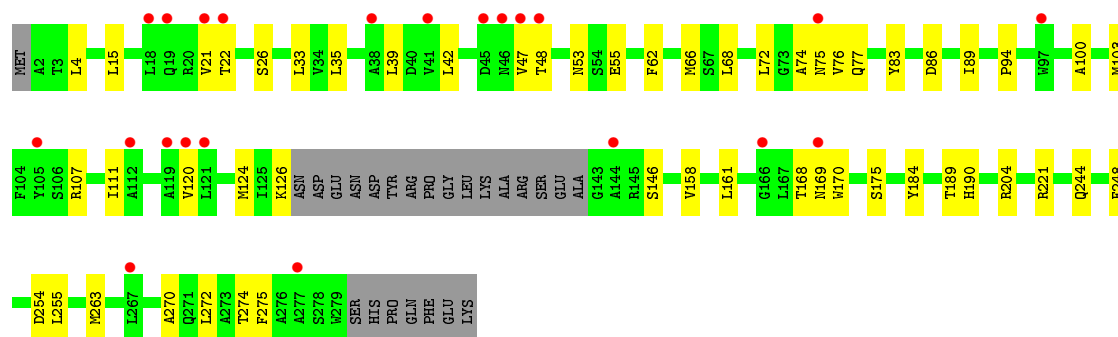
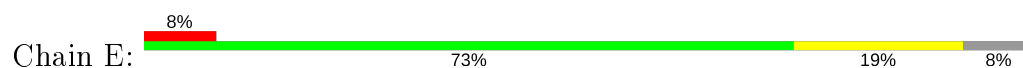


- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

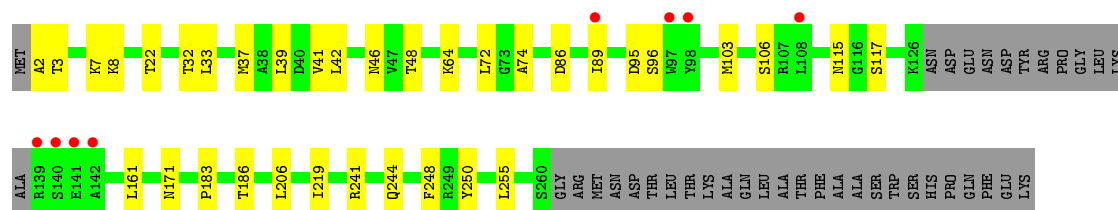




- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



- 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, α , β , γ	108.98Å 108.98Å 323.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.41 48.74 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.35-2.41) 99.5 (48.74-2.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.17-3644	Depositor
R, R_{free}	0.208 , 0.254 0.213 , 0.260	Depositor DCC
R_{free} test set	3802 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11580	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SO4, CU

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	0/2022	0.60	0/2740
1	B	0.52	0/1905	0.69	0/2583
1	C	0.45	0/1948	0.64	0/2637
1	D	0.43	0/1764	0.64	1/2397 (0.0%)
1	E	0.46	0/2002	0.63	0/2719
1	F	0.44	0/1937	0.63	0/2623
All	All	0.46	0/11578	0.64	1/15699 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	ARG	NE-CZ-NH2	-6.79	116.90	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	259	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1993	0	1937	25	1
1	B	1876	0	1839	19	1
1	C	1919	0	1904	23	0
1	D	1735	0	1626	29	0
1	E	1970	0	1916	43	0
1	F	1908	0	1879	26	0
2	A	5	0	0	0	0
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	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	2	0
4	E	5	0	0	1	0
4	F	5	0	0	1	0
5	A	24	0	0	4	0
5	B	26	0	0	0	0
5	C	16	0	0	1	0
5	D	13	0	0	0	0
5	E	21	0	0	2	0
5	F	22	0	0	1	0
All	All	11580	0	11101	162	1

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 7.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:HD2	1:A:116:GLY:O	1.75	0.87
1:E:66:MET:HE2	1:E:76:VAL:HG22	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:GLU:OE2	1:E:190:HIS:NE2	2.13	0.81
1:B:168:THR:CG2	1:C:168:THR:HG22	2.11	0.81
1:B:39:LEU:HD11	1:B:74:ALA:HB2	1.68	0.76
1:D:258:PHE:CZ	1:D:259:ARG:NH1	2.59	0.71
1:A:251:VAL:HG12	1:F:255:LEU:HD22	1.73	0.71
1:E:26:SER:OG	4:E:302:SO4:O3	2.08	0.70
1:E:4:LEU:HD11	1:E:161:LEU:HB2	1.72	0.69
1:F:219:ILE:HD13	1:F:250:TYR:HB2	1.74	0.69
1:B:20:ARG:HG2	1:B:117:SER:HA	1.74	0.69
1:E:53:ASN:HB2	1:E:62:PHE:CE1	2.27	0.69
1:F:22:THR:HG22	1:F:48:THR:HB	1.77	0.67
1:E:22:THR:HB	1:E:120:VAL:HG22	1.77	0.67
1:E:66:MET:CE	1:E:76:VAL:HG22	2.26	0.66
1:A:271:GLN:OE1	5:A:402:HOH:O	2.14	0.66
1:E:33:LEU:HD11	1:E:161:LEU:HD23	1.78	0.66
1:B:168:THR:HG21	1:C:168:THR:HG22	1.78	0.65
1:E:68:LEU:HD21	1:E:169:ASN:HB3	1.78	0.65
4:F:302:SO4:O4	5:F:401:HOH:O	2.13	0.65
1:F:95:ASP:OD1	1:F:95:ASP:N	2.30	0.64
1:C:136:LEU:N	5:C:401:HOH:O	2.31	0.64
1:D:25:PHE:HE1	1:D:32:THR:HA	1.61	0.64
1:C:28:GLY:O	1:C:32:THR:HG23	1.99	0.62
1:E:48:THR:HA	1:E:75:ASN:OD1	1.99	0.62
1:B:20:ARG:NH2	1:B:46:ASN:OD1	2.26	0.61
1:E:35:LEU:HD23	1:E:72:LEU:HD12	1.83	0.60
1:E:86:ASP:HB2	1:E:103:MET:HE1	1.83	0.60
1:A:55:GLU:OE1	1:A:190:HIS:ND1	2.35	0.60
1:E:39:LEU:HD11	1:E:74:ALA:HB2	1.83	0.59
1:A:24:ALA:HB2	1:A:108:LEU:HD11	1.84	0.58
1:A:229:ILE:HD13	1:A:253:LEU:HD21	1.85	0.58
1:F:64:LYS:HE3	1:F:171:ASN:OD1	2.03	0.58
1:B:35:LEU:HD23	1:B:72:LEU:HD12	1.85	0.58
1:D:39:LEU:HD13	1:D:73:GLY:O	2.05	0.56
1:F:8:LYS:NZ	1:F:37:MET:SD	2.78	0.56
1:A:139:ARG:HG2	1:A:144:ALA:HB3	1.87	0.56
1:C:86:ASP:HB2	1:C:103:MET:HE1	1.88	0.56
1:D:124:MET:HB2	1:D:146:SER:OG	2.06	0.56
1:C:20:ARG:HB3	1:C:20:ARG:NH1	2.21	0.55
1:E:189:THR:OG1	5:E:401:HOH:O	2.11	0.55
1:D:36:LYS:HA	1:D:39:LEU:HB2	1.88	0.55
1:E:124:MET:HB2	1:E:146:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:THR:HG23	1:F:72:LEU:HD11	1.90	0.54
1:E:83:TYR:HB3	1:E:89:ILE:HG21	1.88	0.54
1:C:7:LYS:HG2	1:C:151:ALA:O	2.08	0.54
1:E:68:LEU:CD2	1:E:169:ASN:HB3	2.37	0.54
1:F:64:LYS:HD3	1:F:171:ASN:OD1	2.08	0.53
1:A:123:GLY:O	5:A:403:HOH:O	2.18	0.53
1:B:36:LYS:HG2	1:B:167:LEU:HD21	1.91	0.53
1:E:107:ARG:O	1:E:111:ILE:HG13	2.10	0.52
1:F:33:LEU:HD11	1:F:161:LEU:HG	1.92	0.51
1:F:86:ASP:HB3	1:F:89:ILE:HD12	1.92	0.51
5:A:402:HOH:O	1:F:241:ARG:HD2	2.11	0.51
1:A:90:LYS:HD3	1:A:188:LEU:O	2.11	0.50
1:A:138:ALA:N	1:A:140:SER:HG	2.08	0.50
1:D:32:THR:HG23	1:D:72:LEU:HD11	1.94	0.50
1:D:188:LEU:HB3	1:D:193:ILE:HD11	1.93	0.50
1:E:89:ILE:HD11	1:E:100:ALA:HA	1.94	0.49
1:D:229:ILE:HG23	1:D:253:LEU:HD21	1.94	0.49
1:E:168:THR:HA	1:E:170:TRP:CZ3	2.46	0.49
1:D:72:LEU:HD21	1:D:167:LEU:HD22	1.94	0.49
1:F:3:THR:O	1:F:7:LYS:HG3	2.13	0.49
1:C:11:LEU:HD21	1:C:37:MET:HG3	1.93	0.48
1:D:39:LEU:HD22	1:D:44:ARG:HA	1.95	0.48
1:D:25:PHE:CE1	1:D:32:THR:HA	2.45	0.48
1:D:35:LEU:HD11	1:D:49:ALA:HB2	1.95	0.48
1:B:32:THR:HG23	1:B:72:LEU:HD11	1.95	0.48
1:C:26:SER:OG	4:C:302:SO4:O1	2.29	0.48
1:E:94:PRO:HA	1:E:184:TYR:CE1	2.49	0.48
1:F:33:LEU:HD21	1:F:161:LEU:HD23	1.96	0.48
1:D:226:GLU:HA	1:D:229:ILE:HG13	1.96	0.48
1:F:22:THR:HG23	1:F:117:SER:OG	2.14	0.48
1:E:124:MET:HB2	1:E:146:SER:CB	2.44	0.47
1:F:64:LYS:CE	1:F:171:ASN:OD1	2.61	0.47
1:D:157:ASP:O	1:D:161:LEU:HG	2.14	0.47
1:E:126:LYS:HE3	1:E:126:LYS:HB3	1.59	0.47
1:D:39:LEU:HD11	1:D:74:ALA:HB2	1.96	0.47
1:A:8:LYS:O	1:A:12:VAL:HG13	2.13	0.47
1:F:64:LYS:CD	1:F:171:ASN:OD1	2.62	0.47
1:A:39:LEU:HD11	1:A:74:ALA:HB2	1.96	0.47
1:E:39:LEU:HD13	1:E:72:LEU:O	2.15	0.47
1:C:39:LEU:HD11	1:C:74:ALA:HB2	1.96	0.46
1:D:53:ASN:HB3	1:D:80:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:GLN:HA	1:E:248:PHE:O	2.15	0.46
1:E:35:LEU:HD23	1:E:72:LEU:CD1	2.44	0.46
1:E:66:MET:CE	1:E:77:GLN:C	2.84	0.46
1:E:272:LEU:HD23	1:E:275:PHE:HD2	1.80	0.46
1:C:20:ARG:HB3	1:C:20:ARG:HH11	1.80	0.46
1:E:33:LEU:HD22	1:E:158:VAL:HG13	1.98	0.46
1:A:20:ARG:HD2	1:A:116:GLY:C	2.36	0.46
1:E:66:MET:HE2	1:E:76:VAL:CG2	2.40	0.46
1:F:22:THR:HG21	1:F:115:ASN:HD21	1.81	0.46
1:C:52:ALA:HB2	1:C:104:PHE:CE2	2.51	0.45
1:B:2:ALA:HB1	1:B:6:THR:OG1	2.15	0.45
1:E:68:LEU:HD21	1:E:169:ASN:CB	2.46	0.45
1:D:103:MET:HB3	1:D:103:MET:HE3	1.76	0.45
1:B:166:GLY:O	1:B:168:THR:HG23	2.17	0.45
1:C:30:ASP:HB2	4:C:302:SO4:O4	2.16	0.45
1:B:146:SER:O	1:B:150:GLU:HG3	2.17	0.44
1:A:33:LEU:HD21	1:A:161:LEU:HD23	2.00	0.44
1:B:124:MET:HB2	1:B:146:SER:HB3	1.99	0.44
1:F:244:GLN:HA	1:F:248:PHE:O	2.18	0.44
1:D:112:ALA:HB1	1:D:117:SER:HB2	2.00	0.44
1:A:33:LEU:HD11	1:A:161:LEU:HD23	1.99	0.44
1:C:121:LEU:HD22	1:C:147:LEU:HG	1.99	0.44
1:C:7:LYS:HE3	1:C:152:ASP:O	2.17	0.44
1:E:66:MET:HE1	1:E:77:GLN:C	2.38	0.43
1:C:101:LYS:HD2	1:C:101:LYS:HA	1.61	0.43
1:E:221:ARG:HD2	1:E:254:ASP:OD2	2.17	0.43
1:E:263:MET:HG2	1:F:206:LEU:HD23	2.00	0.43
1:F:86:ASP:HB2	1:F:103:MET:HE1	2.00	0.43
1:C:36:LYS:HE3	1:C:40:ASP:OD2	2.18	0.43
1:C:79:THR:OG1	1:C:107:ARG:NH1	2.49	0.43
1:B:218:ASP:N	1:B:218:ASP:OD1	2.52	0.43
1:A:25:PHE:CD2	1:A:69:ALA:HB2	2.54	0.43
1:C:104:PHE:CZ	1:C:108:LEU:HD11	2.54	0.43
1:D:52:ALA:HB1	1:D:81:LEU:HD12	2.01	0.43
1:E:21:VAL:HG22	1:E:47:VAL:HA	2.01	0.43
1:C:103:MET:HE2	1:C:103:MET:HB2	1.76	0.42
1:D:68:LEU:CD2	1:D:170:TRP:HA	2.48	0.42
1:E:204:ARG:NH1	5:E:405:HOH:O	2.52	0.42
1:F:22:THR:CG2	1:F:115:ASN:HD21	2.32	0.42
1:B:221:ARG:HD2	1:B:254:ASP:OD1	2.18	0.42
1:B:224:LEU:HA	1:B:224:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:LEU:O	1:F:46:ASN:ND2	2.42	0.42
1:A:195:GLN:HG3	1:A:246:LEU:O	2.19	0.42
1:E:75:ASN:ND2	1:E:75:ASN:H	2.17	0.42
1:A:44:ARG:NH2	5:A:401:HOH:O	2.13	0.42
1:B:112:ALA:HB1	1:B:117:SER:HB2	2.02	0.42
1:D:224:LEU:HD12	1:D:253:LEU:HD11	2.02	0.42
1:F:2:ALA:O	1:F:7:LYS:HE3	2.19	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.87	0.42
1:D:258:PHE:O	1:D:259:ARG:HB2	2.20	0.42
1:F:39:LEU:HD11	1:F:74:ALA:HB2	2.01	0.42
1:A:202:TYR:CD1	1:A:242:GLN:HG2	2.55	0.42
1:D:39:LEU:CD1	1:D:73:GLY:O	2.68	0.42
1:B:212:ARG:HB2	1:B:223:GLU:HB2	2.02	0.41
1:D:121:LEU:HD23	1:D:147:LEU:HD12	2.02	0.41
1:D:39:LEU:HA	1:D:39:LEU:HD23	1.86	0.41
1:D:39:LEU:HD23	1:D:47:VAL:HB	2.01	0.41
1:D:220:ALA:HB2	1:D:248:PHE:CD1	2.55	0.41
1:E:270:ALA:O	1:E:274:THR:HG23	2.21	0.41
1:A:220:ALA:HB2	1:A:248:PHE:CG	2.55	0.41
1:E:66:MET:HE3	1:E:77:GLN:O	2.21	0.41
1:F:41:VAL:HG12	1:F:42:LEU:HD23	2.03	0.41
1:D:101:LYS:HD3	1:D:101:LYS:HA	1.80	0.41
1:E:15:LEU:HB3	1:E:42:LEU:HD21	2.02	0.41
1:D:94:PRO:HA	1:D:184:TYR:CE2	2.56	0.41
1:E:255:LEU:HD23	1:E:255:LEU:HA	1.86	0.41
1:A:202:TYR:CG	1:A:242:GLN:HG2	2.56	0.41
1:C:145:ARG:NH1	1:C:145:ARG:HG3	2.36	0.41
1:E:68:LEU:HA	1:E:68:LEU:HD23	1.88	0.41
1:B:3:THR:O	1:B:7:LYS:HG3	2.21	0.41
1:F:183:PRO:HD2	1:F:186:THR:OG1	2.21	0.41
1:C:2:ALA:HB1	1:C:6:THR:CG2	2.51	0.40
1:A:64:LYS:O	1:A:68:LEU:HG	2.22	0.40
1:A:145:ARG:NH2	1:A:150:GLU:OE1	2.25	0.40
1:A:200:GLU:HG2	1:A:213:VAL:HG23	2.03	0.40
1:B:214:ARG:NH2	2:B:301:PO4:O3	2.41	0.40
1:E:22:THR:HA	1:E:48:THR:O	2.21	0.40
1:C:33:LEU:HD12	1:C:33:LEU:HA	1.77	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:OD1	1:B:98:TYR:OH[5_555]	1.80	0.40

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	256/286 (90%)	248 (97%)	8 (3%)	0	100	100
1	B	241/286 (84%)	236 (98%)	5 (2%)	0	100	100
1	C	245/286 (86%)	239 (98%)	6 (2%)	0	100	100
1	D	229/286 (80%)	221 (96%)	8 (4%)	0	100	100
1	E	258/286 (90%)	248 (96%)	10 (4%)	0	100	100
1	F	243/286 (85%)	235 (97%)	8 (3%)	0	100	100
All	All	1472/1716 (86%)	1427 (97%)	45 (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	204/236 (86%)	200 (98%)	4 (2%)	55	72
1	B	194/236 (82%)	192 (99%)	2 (1%)	76	87
1	C	201/236 (85%)	198 (98%)	3 (2%)	65	79
1	D	168/236 (71%)	165 (98%)	3 (2%)	59	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	199/236 (84%)	198 (100%)	1 (0%)	88	95
1	F	201/236 (85%)	199 (99%)	2 (1%)	76	87
All	All	1167/1416 (82%)	1152 (99%)	15 (1%)	69	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	90	LYS
1	A	179	SER
1	A	259	ARG
1	B	106	SER
1	B	177	SER
1	C	67	SER
1	C	106	SER
1	C	177	SER
1	D	87	ASP
1	D	145	ARG
1	D	152	ASP
1	E	175	SER
1	F	96	SER
1	F	106	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	E	302	-	4,4,4	0.17	0	6,6,6	0.07	0
4	SO4	C	302	-	4,4,4	0.10	0	6,6,6	0.12	0
4	SO4	A	303	-	4,4,4	0.11	0	6,6,6	0.19	0
4	SO4	F	302	-	4,4,4	0.13	0	6,6,6	0.20	0
4	SO4	B	302	-	4,4,4	0.19	0	6,6,6	0.34	0
2	PO4	A	301	-	4,4,4	1.20	0	6,6,6	0.42	0
2	PO4	B	301	-	4,4,4	2.09	3 (75%)	6,6,6	1.13	0
2	PO4	E	301	-	4,4,4	0.84	0	6,6,6	0.74	0
2	PO4	F	301	-	4,4,4	1.01	0	6,6,6	0.71	0
2	PO4	C	301	-	4,4,4	1.06	0	6,6,6	1.73	2 (33%)
2	PO4	D	301	-	4,4,4	1.07	0	6,6,6	0.51	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	PO4	P-O2	-2.35	1.47	1.54
2	B	301	PO4	P-O1	-2.17	1.45	1.50
2	B	301	PO4	P-O3	-2.16	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	PO4	O4-P-O2	3.01	117.63	107.97
2	C	301	PO4	O4-P-O1	-2.17	102.95	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	302	SO4	1	0
4	C	302	SO4	2	0
4	F	302	SO4	1	0
2	B	301	PO4	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, 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	262/286 (91%)	0.29	11 (4%) 36 34	44, 71, 85, 119	0
1	B	245/286 (85%)	0.18	2 (0%) 86 84	36, 55, 72, 78	0
1	C	249/286 (87%)	0.16	4 (1%) 72 69	39, 63, 80, 96	0
1	D	233/286 (81%)	0.77	26 (11%) 5 4	41, 82, 115, 126	0
1	E	262/286 (91%)	0.61	22 (8%) 11 10	38, 78, 101, 110	0
1	F	247/286 (86%)	0.30	8 (3%) 47 45	39, 65, 83, 99	0
All	All	1498/1716 (87%)	0.38	73 (4%) 29 27	36, 65, 102, 126	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	142	ALA	6.5
1	D	153	PHE	5.6
1	A	143	GLY	5.5
1	D	111	ILE	4.6
1	D	47	VAL	4.1
1	D	105	TYR	4.1
1	D	148	LEU	4.0
1	D	69	ALA	3.8
1	A	139	ARG	3.8
1	D	67	SER	3.6
1	A	141	GLU	3.6
1	D	113	ALA	3.5
1	E	47	VAL	3.2
1	D	32	THR	3.2
1	D	112	ALA	3.2
1	C	97	TRP	3.1
1	D	158	VAL	3.1
1	D	66	MET	3.0
1	E	112	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	41	VAL	3.0
1	E	18	LEU	3.0
1	D	53	ASN	3.0
1	E	144	ALA	3.0
1	D	174	ALA	2.9
1	A	138	ALA	2.9
1	D	50	VAL	2.9
1	D	84	LEU	2.9
1	A	271	GLN	2.8
1	F	98	TYR	2.7
1	E	38	ALA	2.7
1	E	121	LEU	2.7
1	A	268	THR	2.6
1	B	97	TRP	2.6
1	F	97	TRP	2.6
1	C	138	ALA	2.6
1	E	75	ASN	2.6
1	A	140	SER	2.6
1	F	140	SER	2.6
1	D	48	THR	2.6
1	B	143	GLY	2.5
1	E	97	TRP	2.5
1	A	102	LYS	2.5
1	D	169	ASN	2.4
1	A	3	THR	2.4
1	E	119	ALA	2.4
1	F	89	ILE	2.4
1	D	100	ALA	2.3
1	E	48	THR	2.3
1	F	139	ARG	2.3
1	D	73	GLY	2.3
1	C	139	ARG	2.3
1	D	124	MET	2.3
1	E	120	VAL	2.2
1	E	169	ASN	2.2
1	E	166	GLY	2.2
1	D	121	LEU	2.2
1	F	108	LEU	2.2
1	D	42	LEU	2.1
1	F	141	GLU	2.1
1	D	52	ALA	2.1
1	A	142	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	267	LEU	2.1
1	E	46	ASN	2.1
1	C	119	ALA	2.1
1	E	277	ALA	2.1
1	E	45	ASP	2.1
1	D	152	ASP	2.1
1	E	105	TYR	2.1
1	A	89	ILE	2.1
1	D	75	ASN	2.1
1	E	22	THR	2.0
1	E	21	VAL	2.0
1	E	19	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

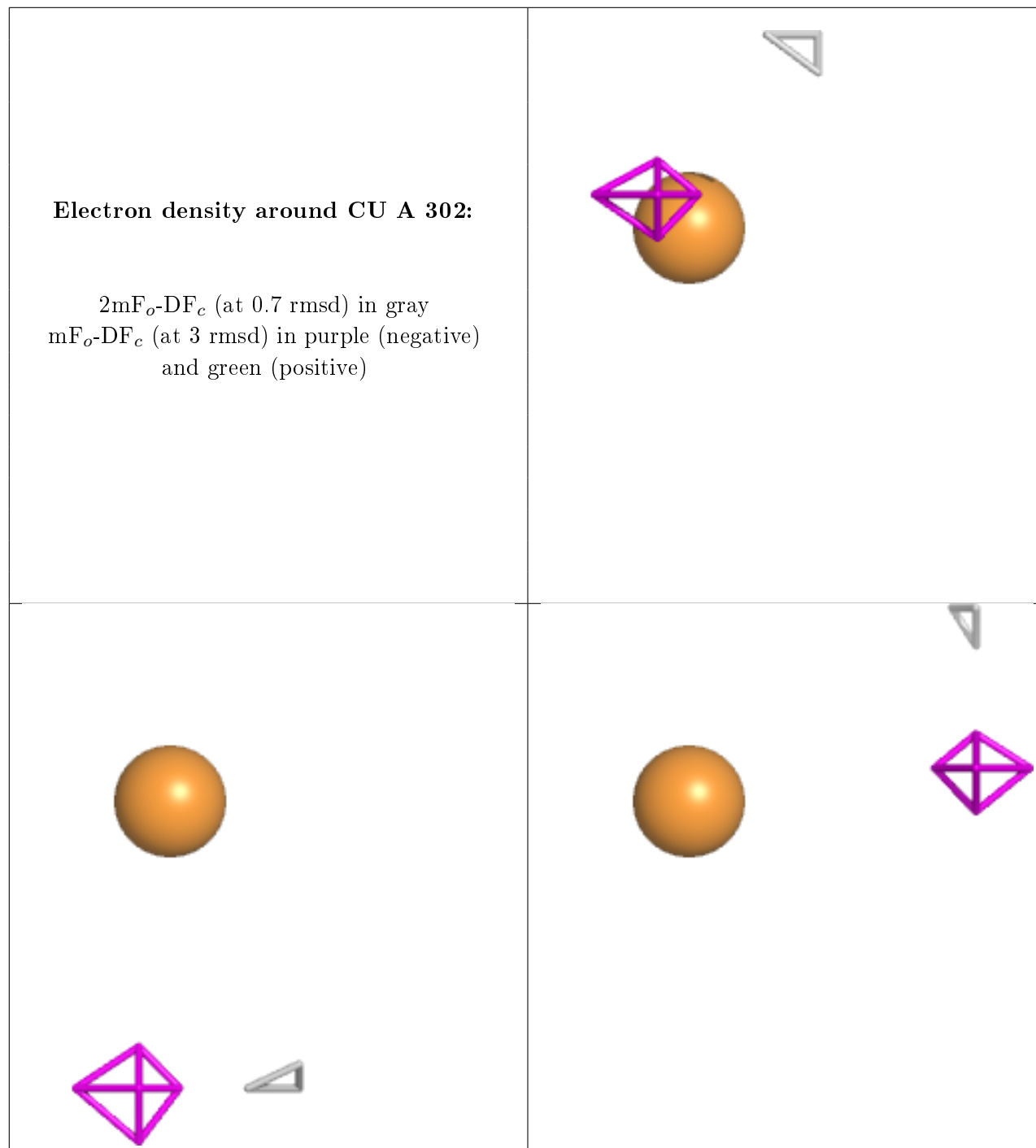
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	303	5/5	0.88	0.25	62,68,71,74	5
4	SO4	E	302	5/5	0.90	0.13	83,84,90,93	5
4	SO4	F	302	5/5	0.92	0.16	63,67,73,74	5
3	CU	A	302	1/1	0.93	0.15	66,66,66,66	1
3	CU	D	302	1/1	0.95	0.17	66,66,66,66	1
4	SO4	B	302	5/5	0.95	0.15	55,55,63,65	5
4	SO4	C	302	5/5	0.96	0.15	68,71,72,74	5
2	PO4	A	301	5/5	0.97	0.18	59,60,68,79	0
2	PO4	B	301	5/5	0.98	0.20	46,50,60,61	0
2	PO4	E	301	5/5	0.98	0.20	49,53,58,68	0
2	PO4	F	301	5/5	0.98	0.20	59,61,67,74	0

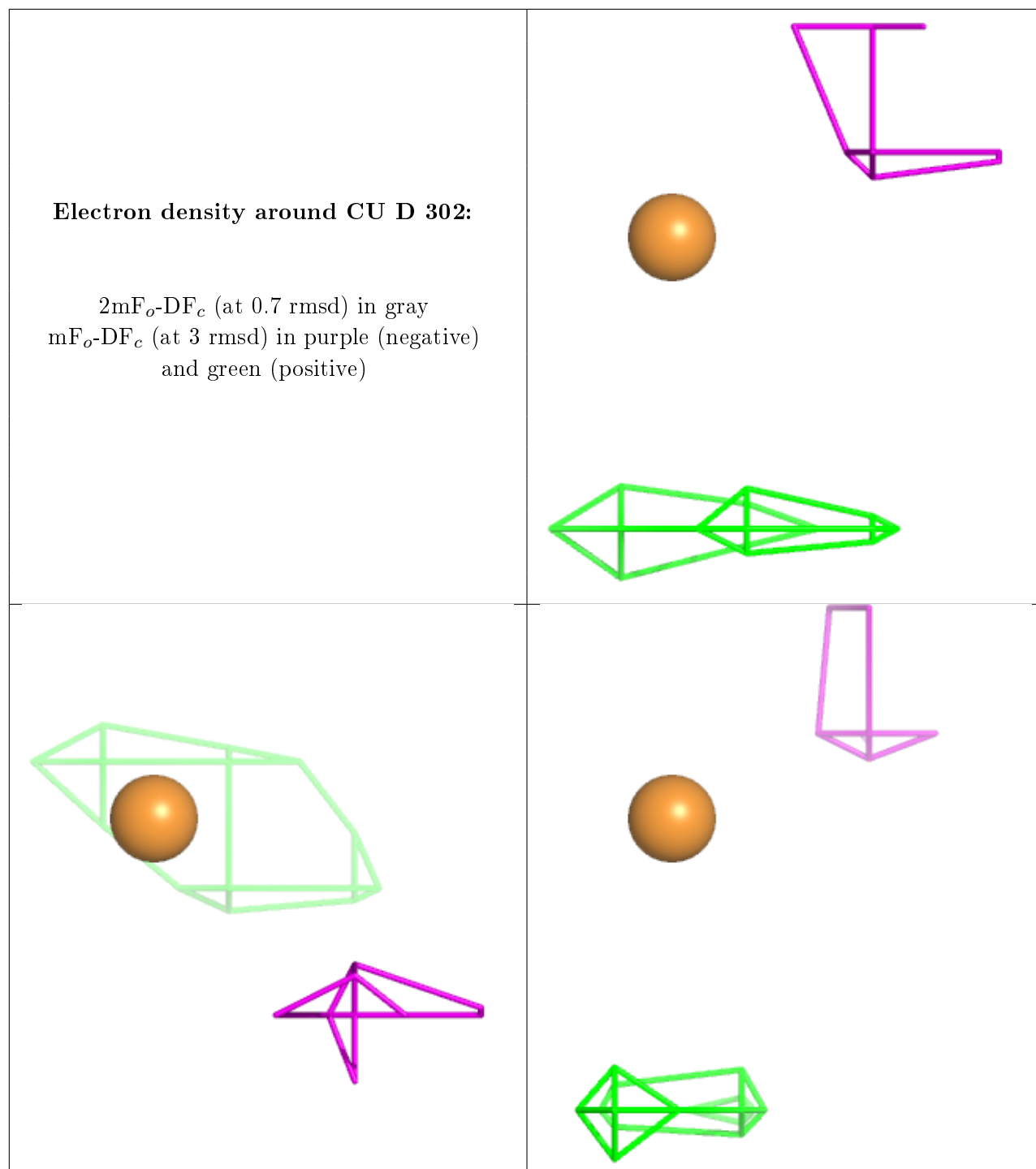
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	C	301	5/5	0.99	0.18	51,56,58,59	0
2	PO4	D	301	5/5	0.99	0.16	51,53,66,67	0

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 ⓘ

There are no such residues in this entry.