



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2022 – 11:28 AM EST

PDB ID : 7TLP
Title : Structure of Atopobium parvulum SufS K235R
Authors : Karunakaran, G.; Couture, J.F.
Deposited on : 2022-01-18
Resolution : 2.99 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 : 2.26
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) : 2.26

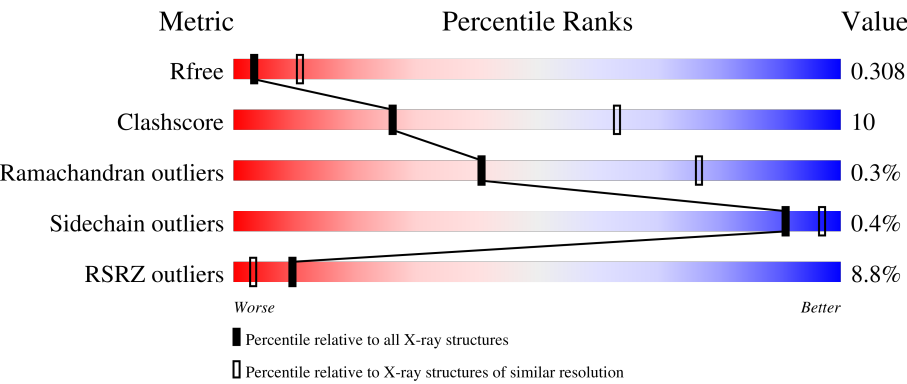
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	447	<div><div>5%</div><div><div></div><div>71%</div><div>15%</div><div>•</div><div>13%</div></div></div>
1	B	447	<div><div>5%</div><div><div></div><div>71%</div><div>17%</div><div></div><div>12%</div></div></div>
1	C	447	<div><div>9%</div><div><div></div><div>68%</div><div>19%</div><div></div><div>12%</div></div></div>
1	D	447	<div><div>8%</div><div><div></div><div>76%</div><div>13%</div><div></div><div>11%</div></div></div>
1	E	447	<div><div>9%</div><div><div></div><div>69%</div><div>19%</div><div></div><div>12%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	447	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLG	A	501	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16670 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 Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	3	0
			2708	1708	475	507	18			
1	B	393	Total	C	N	O	S	0	3	0
			2748	1743	477	511	17			
1	C	392	Total	C	N	O	S	0	3	0
			2741	1730	475	518	18			
1	D	398	Total	C	N	O	S	0	3	0
			2813	1787	491	517	18			
1	E	395	Total	C	N	O	S	0	2	0
			2785	1763	488	516	18			
1	F	396	Total	C	N	O	S	0	3	0
			2755	1748	478	512	17			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP C8W9P2
A	-16	ALA	-	expression tag	UNP C8W9P2
A	-15	SER	-	expression tag	UNP C8W9P2
A	-14	SER	-	expression tag	UNP C8W9P2
A	-13	HIS	-	expression tag	UNP C8W9P2
A	-12	HIS	-	expression tag	UNP C8W9P2
A	-11	HIS	-	expression tag	UNP C8W9P2
A	-10	HIS	-	expression tag	UNP C8W9P2
A	-9	HIS	-	expression tag	UNP C8W9P2
A	-8	HIS	-	expression tag	UNP C8W9P2
A	-7	HIS	-	expression tag	UNP C8W9P2
A	-6	GLU	-	expression tag	UNP C8W9P2
A	-5	ASN	-	expression tag	UNP C8W9P2
A	-4	LEU	-	expression tag	UNP C8W9P2
A	-3	TYR	-	expression tag	UNP C8W9P2
A	-2	PHE	-	expression tag	UNP C8W9P2
A	-1	GLN	-	expression tag	UNP C8W9P2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP C8W9P2
A	90	ALA	ASP	conflict	UNP C8W9P2
A	235	ARG	LYS	engineered mutation	UNP C8W9P2
B	-17	MET	-	initiating methionine	UNP C8W9P2
B	-16	ALA	-	expression tag	UNP C8W9P2
B	-15	SER	-	expression tag	UNP C8W9P2
B	-14	SER	-	expression tag	UNP C8W9P2
B	-13	HIS	-	expression tag	UNP C8W9P2
B	-12	HIS	-	expression tag	UNP C8W9P2
B	-11	HIS	-	expression tag	UNP C8W9P2
B	-10	HIS	-	expression tag	UNP C8W9P2
B	-9	HIS	-	expression tag	UNP C8W9P2
B	-8	HIS	-	expression tag	UNP C8W9P2
B	-7	HIS	-	expression tag	UNP C8W9P2
B	-6	GLU	-	expression tag	UNP C8W9P2
B	-5	ASN	-	expression tag	UNP C8W9P2
B	-4	LEU	-	expression tag	UNP C8W9P2
B	-3	TYR	-	expression tag	UNP C8W9P2
B	-2	PHE	-	expression tag	UNP C8W9P2
B	-1	GLN	-	expression tag	UNP C8W9P2
B	0	GLY	-	expression tag	UNP C8W9P2
B	90	ALA	ASP	conflict	UNP C8W9P2
B	235	ARG	LYS	engineered mutation	UNP C8W9P2
C	-17	MET	-	initiating methionine	UNP C8W9P2
C	-16	ALA	-	expression tag	UNP C8W9P2
C	-15	SER	-	expression tag	UNP C8W9P2
C	-14	SER	-	expression tag	UNP C8W9P2
C	-13	HIS	-	expression tag	UNP C8W9P2
C	-12	HIS	-	expression tag	UNP C8W9P2
C	-11	HIS	-	expression tag	UNP C8W9P2
C	-10	HIS	-	expression tag	UNP C8W9P2
C	-9	HIS	-	expression tag	UNP C8W9P2
C	-8	HIS	-	expression tag	UNP C8W9P2
C	-7	HIS	-	expression tag	UNP C8W9P2
C	-6	GLU	-	expression tag	UNP C8W9P2
C	-5	ASN	-	expression tag	UNP C8W9P2
C	-4	LEU	-	expression tag	UNP C8W9P2
C	-3	TYR	-	expression tag	UNP C8W9P2
C	-2	PHE	-	expression tag	UNP C8W9P2
C	-1	GLN	-	expression tag	UNP C8W9P2
C	0	GLY	-	expression tag	UNP C8W9P2
C	90	ALA	ASP	conflict	UNP C8W9P2

Continued on next page...

Continued from previous page...

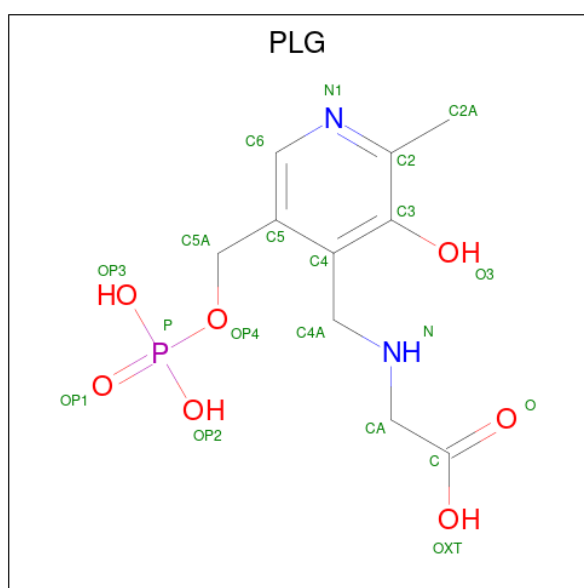
Chain	Residue	Modelled	Actual	Comment	Reference
C	235	ARG	LYS	engineered mutation	UNP C8W9P2
D	-17	MET	-	initiating methionine	UNP C8W9P2
D	-16	ALA	-	expression tag	UNP C8W9P2
D	-15	SER	-	expression tag	UNP C8W9P2
D	-14	SER	-	expression tag	UNP C8W9P2
D	-13	HIS	-	expression tag	UNP C8W9P2
D	-12	HIS	-	expression tag	UNP C8W9P2
D	-11	HIS	-	expression tag	UNP C8W9P2
D	-10	HIS	-	expression tag	UNP C8W9P2
D	-9	HIS	-	expression tag	UNP C8W9P2
D	-8	HIS	-	expression tag	UNP C8W9P2
D	-7	HIS	-	expression tag	UNP C8W9P2
D	-6	GLU	-	expression tag	UNP C8W9P2
D	-5	ASN	-	expression tag	UNP C8W9P2
D	-4	LEU	-	expression tag	UNP C8W9P2
D	-3	TYR	-	expression tag	UNP C8W9P2
D	-2	PHE	-	expression tag	UNP C8W9P2
D	-1	GLN	-	expression tag	UNP C8W9P2
D	0	GLY	-	expression tag	UNP C8W9P2
D	90	ALA	ASP	conflict	UNP C8W9P2
D	235	ARG	LYS	engineered mutation	UNP C8W9P2
E	-17	MET	-	initiating methionine	UNP C8W9P2
E	-16	ALA	-	expression tag	UNP C8W9P2
E	-15	SER	-	expression tag	UNP C8W9P2
E	-14	SER	-	expression tag	UNP C8W9P2
E	-13	HIS	-	expression tag	UNP C8W9P2
E	-12	HIS	-	expression tag	UNP C8W9P2
E	-11	HIS	-	expression tag	UNP C8W9P2
E	-10	HIS	-	expression tag	UNP C8W9P2
E	-9	HIS	-	expression tag	UNP C8W9P2
E	-8	HIS	-	expression tag	UNP C8W9P2
E	-7	HIS	-	expression tag	UNP C8W9P2
E	-6	GLU	-	expression tag	UNP C8W9P2
E	-5	ASN	-	expression tag	UNP C8W9P2
E	-4	LEU	-	expression tag	UNP C8W9P2
E	-3	TYR	-	expression tag	UNP C8W9P2
E	-2	PHE	-	expression tag	UNP C8W9P2
E	-1	GLN	-	expression tag	UNP C8W9P2
E	0	GLY	-	expression tag	UNP C8W9P2
E	90	ALA	ASP	conflict	UNP C8W9P2
E	235	ARG	LYS	engineered mutation	UNP C8W9P2
F	-17	MET	-	initiating methionine	UNP C8W9P2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	ALA	-	expression tag	UNP C8W9P2
F	-15	SER	-	expression tag	UNP C8W9P2
F	-14	SER	-	expression tag	UNP C8W9P2
F	-13	HIS	-	expression tag	UNP C8W9P2
F	-12	HIS	-	expression tag	UNP C8W9P2
F	-11	HIS	-	expression tag	UNP C8W9P2
F	-10	HIS	-	expression tag	UNP C8W9P2
F	-9	HIS	-	expression tag	UNP C8W9P2
F	-8	HIS	-	expression tag	UNP C8W9P2
F	-7	HIS	-	expression tag	UNP C8W9P2
F	-6	GLU	-	expression tag	UNP C8W9P2
F	-5	ASN	-	expression tag	UNP C8W9P2
F	-4	LEU	-	expression tag	UNP C8W9P2
F	-3	TYR	-	expression tag	UNP C8W9P2
F	-2	PHE	-	expression tag	UNP C8W9P2
F	-1	GLN	-	expression tag	UNP C8W9P2
F	0	GLY	-	expression tag	UNP C8W9P2
F	90	ALA	ASP	conflict	UNP C8W9P2
F	235	ARG	LYS	engineered mutation	UNP C8W9P2

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-P YRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: $C_{10}H_{15}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

Continued on next page...

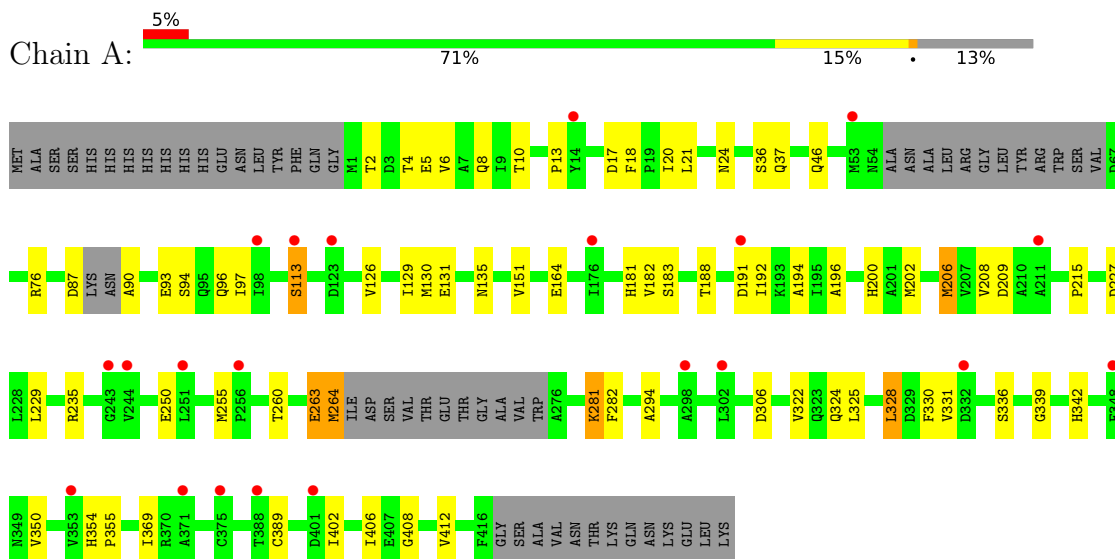
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	E	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	F	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

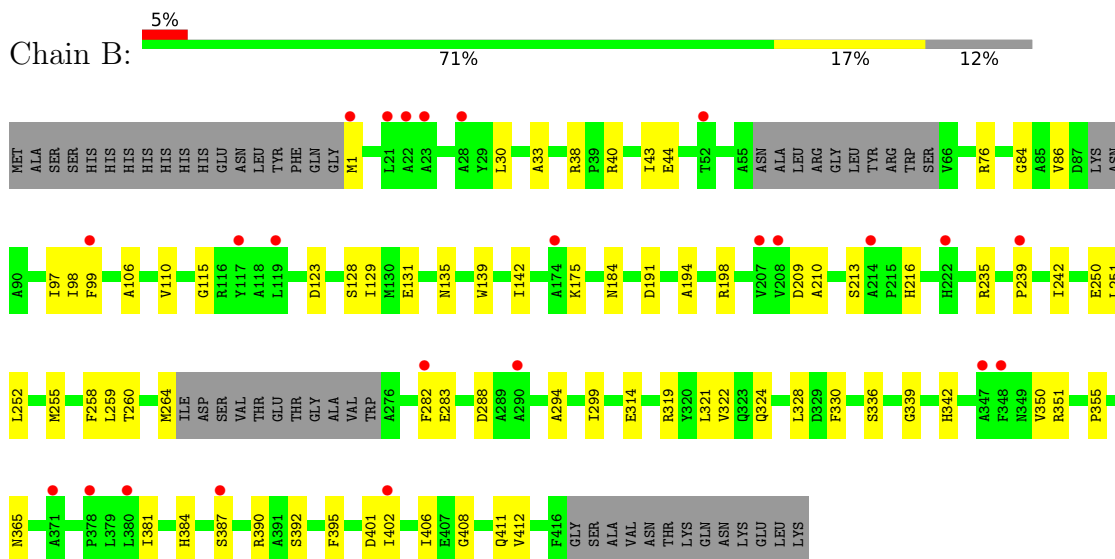
3 Residue-property plots [i](#)

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.

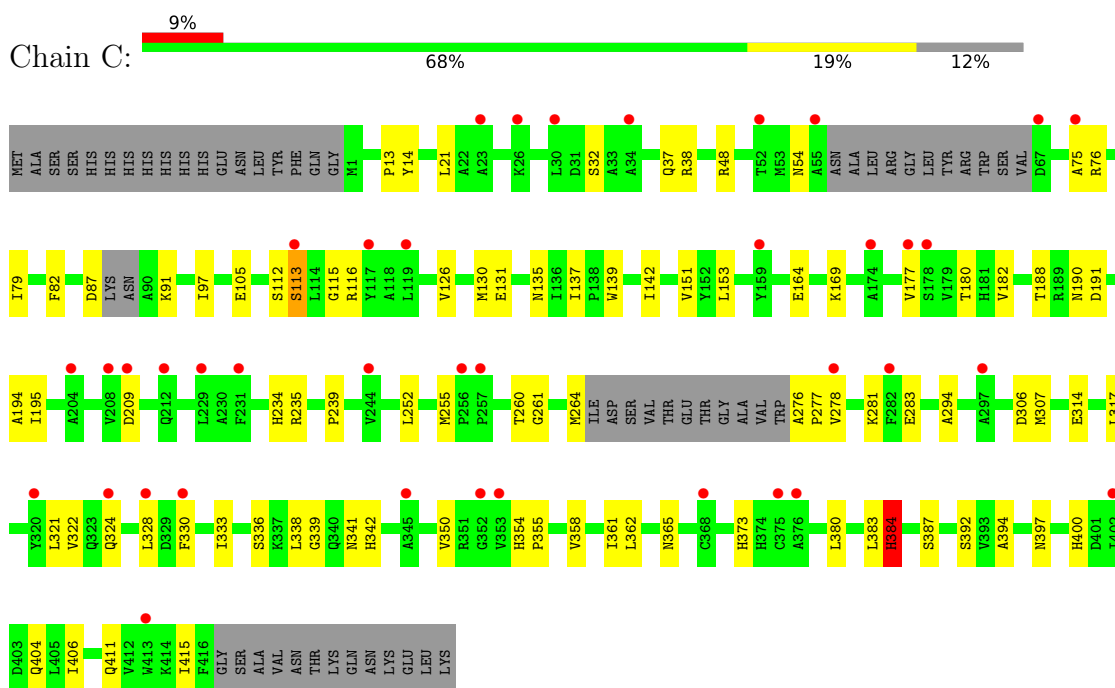
• Molecule 1: Cysteine desulfurase



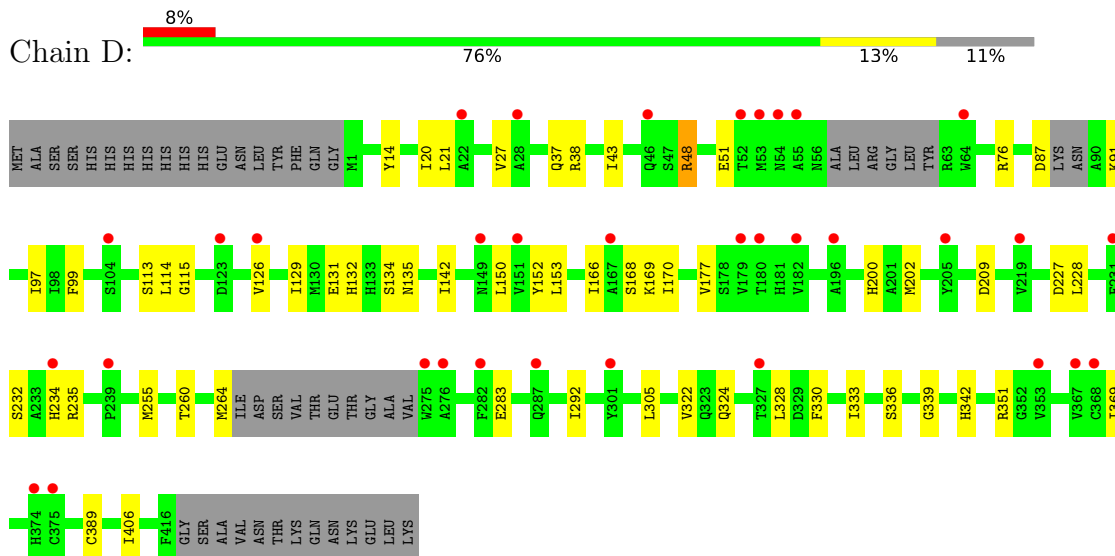
• Molecule 1: Cysteine desulfurase



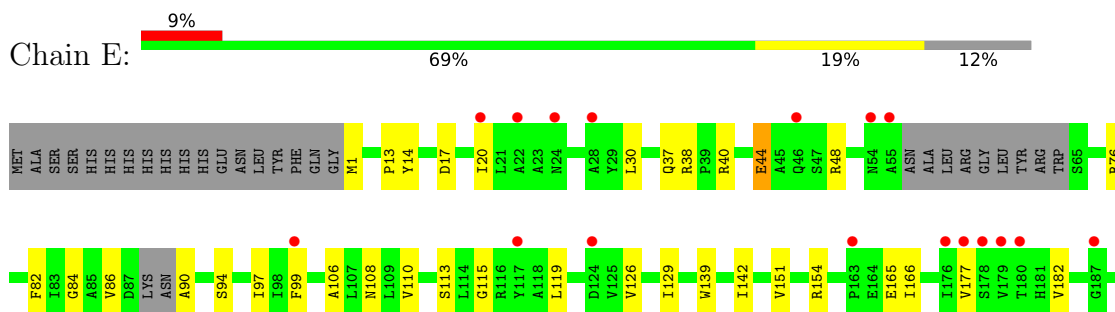
• Molecule 1: Cysteine desulfurase

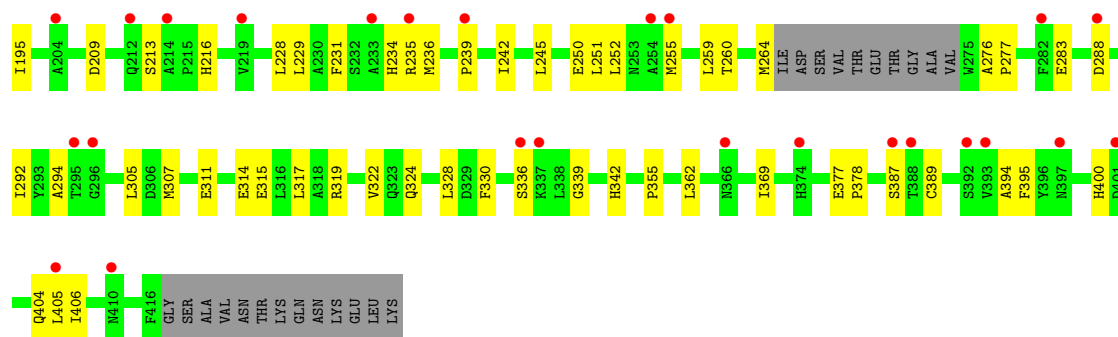


- Molecule 1: Cysteine desulfurase

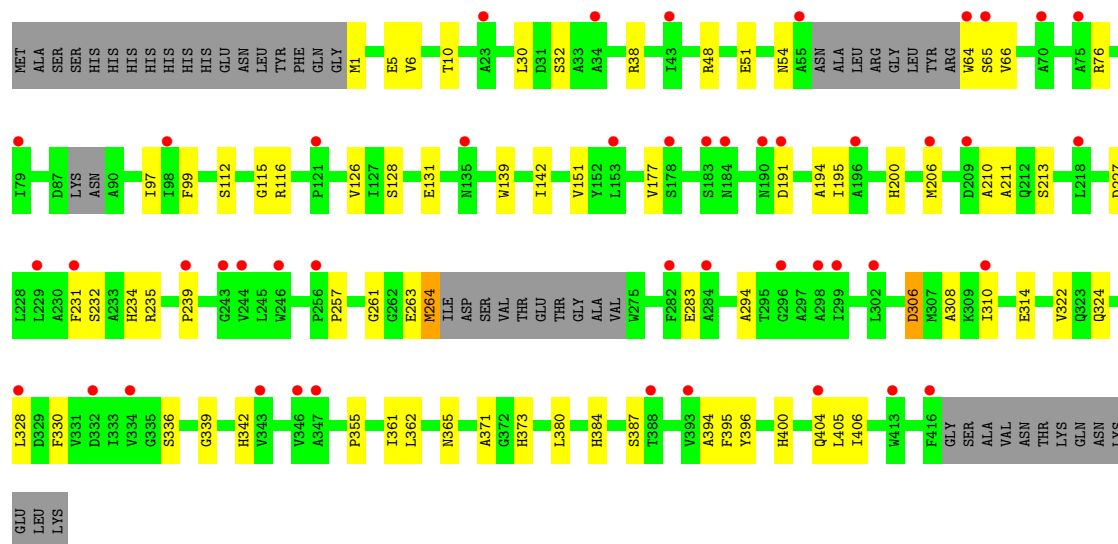
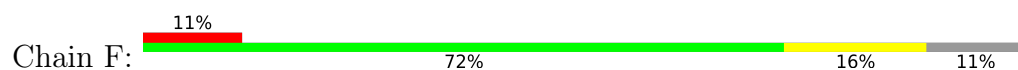


- Molecule 1: Cysteine desulfurase





● Molecule 1: Cysteine desulfurase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.74Å 159.26Å 178.07Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	38.86 – 2.99 38.86 – 2.99	Depositor EDS
% Data completeness (in resolution range)	96.3 (38.86-2.99) 95.6 (38.86-2.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.237 , 0.309 0.236 , 0.308	Depositor DCC
R_{free} test set	2005 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.448 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.450 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.449 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.440 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.457 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16670	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: PLG

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	0.59	1/2769 (0.0%)	0.77	5/3797 (0.1%)
1	B	0.55	0/2810	0.69	0/3853
1	C	0.55	0/2801	0.72	3/3840 (0.1%)
1	D	0.57	0/2878	0.74	2/3944 (0.1%)
1	E	0.59	1/2844 (0.0%)	0.74	5/3892 (0.1%)
1	F	0.54	0/2819	0.75	2/3870 (0.1%)
All	All	0.57	2/16921 (0.0%)	0.74	17/23196 (0.1%)

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	A	0	1
1	C	0	1
1	F	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	44	GLU	CD-OE2	5.59	1.31	1.25
1	A	264	MET	CG-SD	5.46	1.95	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	264	MET	N-CA-C	-12.19	78.09	111.00
1	A	264	MET	CA-CB-CG	-10.81	94.93	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	MET	CG-SD-CE	-9.54	84.93	100.20
1	D	48	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	D	27	VAL	CG1-CB-CG2	8.00	123.69	110.90
1	F	264	MET	CG-SD-CE	-7.61	88.02	100.20
1	E	44	GLU	OE1-CD-OE2	7.33	132.10	123.30
1	A	281	LYS	CD-CE-NZ	-6.14	97.57	111.70
1	A	328	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	E	119	LEU	C-N-CA	5.49	135.42	121.70
1	E	44	GLU	CB-CG-CD	-5.47	99.42	114.20
1	E	44	GLU	CA-CB-CG	5.41	125.30	113.40
1	C	384	HIS	N-CA-CB	-5.39	100.91	110.60
1	A	206	MET	CG-SD-CE	5.21	108.54	100.20
1	C	321	LEU	CB-CG-CD1	5.19	119.83	111.00
1	C	321	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	E	90	ALA	C-N-CA	-5.10	108.96	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	GLU	Peptide
1	C	384	HIS	Sidechain
1	F	263	GLU	Peptide

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	2708	0	2413	59	0
1	B	2748	0	2495	57	0
1	C	2741	0	2465	67	0
1	D	2813	0	2575	40	0
1	E	2785	0	2550	68	0
1	F	2755	0	2485	52	0
2	A	20	0	12	7	0
2	B	20	0	12	4	0
2	C	20	0	12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	20	0	12	4	0
2	E	20	0	12	4	0
2	F	20	0	12	3	0
All	All	16670	0	15055	329	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 10.

All (329) 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:260:THR:HG22	1:A:264:MET:HE1	1.34	1.08
1:E:40:ARG:NH1	1:E:44:GLU:OE2	1.88	1.07
1:E:1:MET:HG2	1:E:319:ARG:HH21	1.36	0.88
1:A:235:ARG:NH2	2:A:501:PLG:H4A2	1.90	0.87
1:E:324:GLN:HG2	1:E:406:ILE:HG13	1.56	0.86
1:A:20:ILE:HG21	1:A:37:GLN:HE21	1.43	0.84
1:B:384:HIS:ND1	1:E:44:GLU:OE1	2.10	0.83
1:A:260:THR:HG22	1:A:264:MET:CE	2.09	0.82
1:D:324:GLN:HG2	1:D:406:ILE:HG13	1.60	0.82
1:C:261:GLY:H	1:C:264:MET:HE2	1.44	0.82
1:A:76:ARG:HA	1:A:97:ILE:HD11	1.62	0.81
1:A:20:ILE:HG21	1:A:37:GLN:NE2	1.96	0.80
1:C:324:GLN:HG2	1:C:406:ILE:HG13	1.66	0.78
1:A:6:VAL:O	1:A:10:THR:OG1	2.01	0.78
1:A:324:GLN:HG2	1:A:406:ILE:HG13	1.66	0.77
1:C:21:LEU:HD21	1:C:37:GLN:HG3	1.68	0.73
1:A:20:ILE:O	1:A:24:ASN:ND2	2.21	0.73
1:D:200:HIS:HE1	1:D:227:ASP:OD2	1.71	0.72
1:A:46:GLN:HB2	1:A:294:ALA:HB2	1.72	0.71
1:E:76:ARG:HA	1:E:97:ILE:HD11	1.73	0.71
1:B:239:PRO:HG3	1:B:294:ALA:HB3	1.74	0.70
1:B:322:VAL:HG11	1:B:339:GLY:HA3	1.74	0.70
1:C:235:ARG:NH2	2:C:501:PLG:H4A2	2.06	0.70
1:E:1:MET:HG2	1:E:319:ARG:NH2	2.06	0.69
1:F:361:ILE:O	1:F:365:ASN:ND2	2.26	0.69
1:D:20:ILE:HG21	1:D:37:GLN:NE2	2.08	0.69
1:B:314:GLU:OE2	1:B:395:PHE:N	2.27	0.68
1:C:278:VAL:HG22	1:C:281:LYS:HD3	1.73	0.68
1:D:260:THR:HA	1:D:264:MET:SD	2.35	0.67
1:F:324:GLN:HG2	1:F:406:ILE:HG13	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:THR:HA	1:E:264:MET:SD	2.35	0.67
1:D:322:VAL:HG11	1:D:339:GLY:HA3	1.76	0.67
1:F:355:PRO:HG2	1:F:387:SER:HB3	1.77	0.67
1:A:200:HIS:HE1	1:A:227:ASP:OD2	1.78	0.66
1:F:235:ARG:NH2	2:F:501:PLG:H4A2	2.11	0.66
1:A:260:THR:CG2	1:A:264:MET:HE1	2.18	0.65
1:C:112:SER:O	1:C:116:ARG:HG3	1.96	0.65
1:F:264:MET:O	1:F:264:MET:HG3	1.97	0.65
1:A:235:ARG:HH22	2:A:501:PLG:H4A2	1.60	0.64
1:A:250:GLU:OE2	1:B:198:ARG:NH1	2.29	0.64
1:C:54:ASN:ND2	1:E:37:GLN:OE1	2.27	0.64
1:A:164:GLU:N	1:A:164:GLU:OE1	2.30	0.64
1:A:2:THR:OG1	1:A:5:GLU:HG3	1.97	0.64
1:F:191:ASP:OD2	1:F:194:ALA:HB2	1.98	0.64
1:F:322:VAL:HG21	1:F:339:GLY:HA3	1.79	0.64
1:F:64:TRP:C	1:F:66:VAL:H	2.01	0.63
1:E:38:ARG:NH2	1:E:234:HIS:HB2	2.12	0.63
1:C:164:GLU:N	1:C:164:GLU:OE1	2.30	0.63
1:E:126:VAL:HB	1:E:177:VAL:HG22	1.81	0.63
1:F:126:VAL:HB	1:F:177:VAL:HG22	1.81	0.63
1:E:400:HIS:O	1:E:404:GLN:HG3	1.99	0.63
1:C:126:VAL:HB	1:C:177:VAL:HG22	1.81	0.63
1:B:235:ARG:NH2	2:B:501:PLG:H4A2	2.14	0.62
1:C:130:MET:CE	1:C:190:ASN:HD21	2.11	0.62
1:D:328:LEU:HD13	1:D:330:PHE:CZ	2.34	0.62
1:F:314:GLU:OE2	1:F:394:ALA:HA	1.98	0.62
1:C:48:ARG:HG3	1:F:384:HIS:NE2	2.14	0.62
1:B:184:ASN:O	1:B:390:ARG:NH1	2.30	0.61
1:B:235:ARG:CZ	2:B:501:PLG:H4A2	2.29	0.61
1:A:322:VAL:HG21	1:A:339:GLY:HA3	1.82	0.61
1:D:150:LEU:HD22	1:D:152:TYR:CE1	2.36	0.61
1:E:154:ARG:N	1:E:165:GLU:OE1	2.33	0.61
1:E:336:SER:O	1:E:342:HIS:NE2	2.28	0.61
1:F:235:ARG:HH22	2:F:501:PLG:P	2.24	0.60
1:C:235:ARG:HH22	2:C:501:PLG:P	2.23	0.60
1:F:76:ARG:HA	1:F:97:ILE:HD11	1.83	0.60
1:B:216:HIS:ND1	1:B:314:GLU:OE1	2.34	0.60
2:A:501:PLG:O3	2:A:501:PLG:N	2.33	0.59
1:A:181:HIS:CD2	1:A:192:ILE:HG13	2.37	0.59
1:F:128:SER:O	1:F:131:GLU:HG2	2.02	0.59
1:F:112:SER:O	1:F:116:ARG:HG3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:PHE:HD1	1:B:350:VAL:HG13	1.68	0.58
1:B:76:ARG:HA	1:B:97:ILE:HD11	1.85	0.58
1:C:38:ARG:HH12	1:C:234:HIS:HB2	1.68	0.58
1:D:114:LEU:HD13	1:D:255:MET:HE2	1.86	0.58
1:F:64:TRP:O	1:F:66:VAL:N	2.37	0.58
1:F:310:ILE:O	1:F:314:GLU:HG3	2.04	0.57
1:C:261:GLY:H	1:C:264:MET:CE	2.12	0.57
1:F:6:VAL:O	1:F:10:THR:OG1	2.22	0.57
1:A:196:ALA:HA	1:A:206:MET:HE2	1.85	0.57
1:B:260:THR:HA	1:B:264:MET:SD	2.45	0.57
1:A:130:MET:HE3	1:A:183:SER:HB2	1.87	0.56
1:B:384:HIS:HB3	1:E:44:GLU:OE1	2.06	0.56
1:E:314:GLU:OE2	1:E:395:PHE:N	2.38	0.56
1:C:361:ILE:O	1:C:365:ASN:ND2	2.38	0.56
1:D:235:ARG:CZ	2:D:501:PLG:H4A2	2.35	0.56
1:A:17:ASP:OD1	1:D:351:ARG:HD3	2.04	0.56
1:A:130:MET:CE	1:A:183:SER:HB2	2.36	0.56
1:E:182:VAL:HG23	1:E:213:SER:HB3	1.87	0.56
1:D:166:ILE:HG23	1:D:170:ILE:HD12	1.88	0.56
1:F:314:GLU:OE2	1:F:395:PHE:N	2.38	0.56
1:A:36:SER:OG	1:A:235:ARG:O	2.24	0.56
1:E:369:ILE:HD12	1:E:389:CYS:HB3	1.88	0.56
1:F:116:ARG:NH2	1:F:257:PRO:O	2.39	0.56
1:D:126:VAL:HB	1:D:177:VAL:HG22	1.89	0.55
1:D:322:VAL:HG11	1:D:339:GLY:CA	2.36	0.55
1:A:209:ASP:OD2	2:A:501:PLG:N1	2.39	0.55
1:F:324:GLN:CG	1:F:406:ILE:HG13	2.37	0.55
1:D:76:ARG:HA	1:D:97:ILE:HD11	1.88	0.55
1:F:195:ILE:C	1:F:206:MET:HE3	2.27	0.55
1:E:377:GLU:HB2	1:E:378:PRO:HD3	1.89	0.55
1:A:76:ARG:NH1	1:A:97:ILE:O	2.40	0.55
1:A:330:PHE:HD2	1:A:350:VAL:HG13	1.72	0.55
1:E:166:ILE:HD12	1:E:195:ILE:HG12	1.88	0.55
1:B:381:ILE:O	1:E:48:ARG:NH1	2.40	0.54
1:B:139:TRP:HA	1:B:142:ILE:HG22	1.89	0.54
1:A:76:ARG:HB3	1:A:94:SER:HB2	1.90	0.54
1:E:235:ARG:CZ	2:E:501:PLG:H4A2	2.37	0.54
1:A:191:ASP:OD2	1:A:194:ALA:HB2	2.06	0.54
1:E:264:MET:O	1:E:264:MET:HG3	2.06	0.54
1:F:306:ASP:OD2	1:F:308:ALA:HB3	2.06	0.54
1:F:336:SER:O	1:F:342:HIS:NE2	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:ILE:HD12	1:D:389:CYS:HB3	1.90	0.54
1:E:315:GLU:O	1:E:319:ARG:HB2	2.08	0.53
1:B:365:ASN:ND2	1:B:411:GLN:OE1	2.30	0.53
1:B:322:VAL:HG11	1:B:339:GLY:CA	2.38	0.53
1:A:13:PRO:O	1:D:351:ARG:HD2	2.08	0.53
1:C:13:PRO:HG2	1:C:14:TYR:CE2	2.43	0.53
1:E:235:ARG:NH2	2:E:501:PLG:H4A2	2.21	0.53
1:F:261:GLY:H	1:F:264:MET:HE1	1.74	0.53
1:C:322:VAL:HG11	1:C:339:GLY:HA3	1.91	0.53
1:B:351:ARG:HD3	1:E:17:ASP:OD2	2.07	0.53
1:C:373:HIS:HA	1:C:380:LEU:HD22	1.91	0.53
1:C:139:TRP:HA	1:C:142:ILE:HG22	1.90	0.52
1:E:216:HIS:O	1:E:311:GLU:HG3	2.09	0.52
1:F:1:MET:N	1:F:5:GLU:OE2	2.37	0.52
1:F:328:LEU:HD13	1:F:330:PHE:CZ	2.44	0.52
1:B:1:MET:N	1:B:319:ARG:HH22	2.07	0.52
1:A:336:SER:O	1:A:342:HIS:NE2	2.30	0.52
1:F:322:VAL:HG21	1:F:339:GLY:CA	2.38	0.52
1:B:251:LEU:O	1:B:255:MET:HG3	2.09	0.52
1:B:328:LEU:HD13	1:B:330:PHE:CZ	2.44	0.52
1:A:208:VAL:HG21	1:A:229:LEU:HD12	1.91	0.52
1:B:324:GLN:HB3	1:B:406:ILE:HG13	1.93	0.51
1:F:139:TRP:HA	1:F:142:ILE:HG22	1.92	0.51
1:C:115:GLY:HA3	1:C:142:ILE:HG12	1.93	0.51
1:F:32:SER:HG	1:F:396:TYR:HH	1.54	0.51
1:F:355:PRO:HB2	1:F:371:ALA:HB1	1.93	0.51
1:C:264:MET:HB2	1:C:281:LYS:HA	1.93	0.50
1:A:369:ILE:HD12	1:A:389:CYS:HB3	1.92	0.50
1:A:126:VAL:HA	1:A:151:VAL:O	2.12	0.50
1:C:260:THR:HA	1:C:264:MET:HE1	1.92	0.50
1:C:264:MET:O	1:C:264:MET:HG3	2.10	0.50
1:F:38:ARG:HH11	1:F:234:HIS:HB2	1.75	0.50
1:C:76:ARG:NH1	1:C:97:ILE:O	2.44	0.50
1:D:48:ARG:HA	1:D:51:GLU:HB2	1.93	0.50
1:A:324:GLN:CG	1:A:406:ILE:HG13	2.40	0.50
1:C:314:GLU:OE2	1:C:394:ALA:HA	2.12	0.50
1:B:40:ARG:NH1	1:B:44:GLU:OE1	2.44	0.49
1:F:200:HIS:HE1	1:F:227:ASP:OD1	1.95	0.49
1:D:202:MET:CE	1:E:250:GLU:HG2	2.42	0.49
1:C:21:LEU:CD2	1:C:37:GLN:HG3	2.42	0.49
1:D:209:ASP:OD2	2:D:501:PLG:N1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ARG:NH2	2:D:501:PLG:H4A2	2.27	0.49
1:E:126:VAL:HG13	1:E:151:VAL:HG12	1.95	0.49
1:B:30:LEU:HD21	1:B:401:ASP:HB3	1.94	0.49
1:A:328:LEU:HD23	1:A:330:PHE:CZ	2.48	0.49
1:C:191:ASP:O	1:C:195:ILE:HG12	2.12	0.49
1:D:328:LEU:HD13	1:D:330:PHE:HZ	1.75	0.49
1:E:314:GLU:OE2	1:E:394:ALA:HA	2.13	0.49
1:C:239:PRO:HG3	1:C:294:ALA:HB3	1.94	0.48
1:F:126:VAL:HG22	1:F:151:VAL:HB	1.95	0.48
1:E:84:GLY:O	1:E:86:VAL:HG22	2.13	0.48
1:E:38:ARG:HH22	1:E:234:HIS:HB2	1.76	0.48
1:A:113[B]:SER:OG	1:A:255:MET:HB3	2.13	0.48
1:A:202:MET:CE	1:B:250:GLU:HG2	2.43	0.48
1:B:1:MET:H1	1:B:319:ARG:NH2	2.12	0.48
1:C:105:GLU:HG3	1:E:259:LEU:HD21	1.96	0.48
1:E:115:GLY:HA3	1:E:142:ILE:HG12	1.94	0.48
1:F:195:ILE:HG22	1:F:206:MET:CE	2.44	0.48
1:A:260:THR:HA	1:A:264:MET:HE3	1.95	0.48
1:A:281:LYS:HE3	1:A:282:PHE:CZ	2.48	0.48
1:C:75:ALA:O	1:C:79:ILE:HG12	2.13	0.48
1:D:228:LEU:HD11	1:D:255:MET:CE	2.44	0.48
1:B:384:HIS:CG	1:E:44:GLU:OE1	2.67	0.48
1:E:362:LEU:HD12	1:E:369:ILE:HD13	1.95	0.48
1:B:258:PHE:CD2	1:B:259:LEU:HD23	2.49	0.47
1:E:20:ILE:HG21	1:E:37:GLN:OE1	2.13	0.47
1:E:99:PHE:N	1:E:283:GLU:OE2	2.34	0.47
1:D:37:GLN:NE2	1:D:37:GLN:HA	2.29	0.47
1:E:13:PRO:HG2	1:E:14:TYR:CE2	2.49	0.47
1:A:215:PRO:HG2	1:A:235:ARG:HB3	1.95	0.47
1:B:242:ILE:HD11	1:B:288:ASP:HB3	1.97	0.47
1:A:196:ALA:HA	1:A:206:MET:CE	2.44	0.47
1:B:191:ASP:OD1	1:B:194:ALA:HB2	2.15	0.47
1:B:209:ASP:OD2	2:B:501:PLG:N1	2.48	0.47
1:F:64:TRP:C	1:F:66:VAL:N	2.68	0.47
1:B:99:PHE:N	1:B:283:GLU:OE2	2.38	0.47
1:B:131:GLU:CD	1:B:135:ASN:HD22	2.17	0.47
1:C:330:PHE:HD1	1:C:350:VAL:HG13	1.80	0.47
1:F:99:PHE:N	1:F:283:GLU:OE2	2.39	0.47
1:B:106:ALA:O	1:B:110:VAL:HG23	2.16	0.46
1:C:82:PHE:HZ	1:C:307:MET:HE1	1.79	0.46
1:B:252:LEU:HD23	1:B:255:MET:CE	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:HH22	1:C:283:GLU:CD	2.18	0.46
1:D:38:ARG:HB2	1:D:43:ILE:HD11	1.96	0.46
1:B:40:ARG:HH11	1:B:44:GLU:CD	2.18	0.46
1:E:322:VAL:HG21	1:E:339:GLY:CA	2.45	0.46
1:A:235:ARG:HH12	2:A:501:PLG:P	2.39	0.46
1:E:129:ILE:HA	1:E:129:ILE:HD12	1.79	0.46
1:F:400:HIS:O	1:F:404:GLN:HG3	2.16	0.46
1:B:384:HIS:HB3	1:E:44:GLU:CD	2.36	0.46
1:C:354:HIS:O	1:C:358:VAL:HG23	2.16	0.46
1:F:232:SER:HB2	1:F:235:ARG:NH1	2.30	0.46
1:A:408:GLY:O	1:A:412:VAL:HG23	2.16	0.46
1:E:30:LEU:HD13	1:E:405:LEU:HD12	1.97	0.46
1:C:260:THR:O	1:E:108:ASN:ND2	2.35	0.45
1:E:209:ASP:OD2	2:E:501:PLG:N1	2.49	0.45
1:E:14:TYR:CE1	1:E:305:LEU:HD22	2.51	0.45
1:C:328:LEU:HD22	1:C:330:PHE:CE2	2.52	0.45
1:D:87:ASP:N	1:D:91:LYS:O	2.40	0.45
2:E:501:PLG:O3	2:E:501:PLG:N	2.49	0.45
1:B:115:GLY:HA3	1:B:142:ILE:HG12	1.99	0.45
1:C:182:VAL:HA	1:C:188:THR:O	2.17	0.45
1:C:235:ARG:NH1	1:C:235:ARG:HG3	2.32	0.45
1:F:239:PRO:HG3	1:F:294:ALA:HB3	1.98	0.45
1:D:14:TYR:CE1	1:D:305:LEU:HD22	2.52	0.45
1:D:228:LEU:HD11	1:D:255:MET:HE1	1.98	0.45
1:A:131:GLU:CD	1:A:135:ASN:HD22	2.19	0.45
1:B:84:GLY:O	1:B:86:VAL:HG22	2.17	0.45
1:E:166:ILE:CD1	1:E:195:ILE:HG12	2.47	0.45
1:A:235:ARG:NH2	2:A:501:PLG:HA2	2.32	0.45
1:C:400:HIS:O	1:C:404:GLN:HG3	2.17	0.45
1:B:1:MET:N	1:B:319:ARG:NH2	2.64	0.45
1:C:32:SER:N	1:C:392:SER:HB2	2.32	0.45
1:D:99:PHE:CZ	1:D:292:ILE:HG23	2.52	0.45
1:E:76:ARG:NH2	1:E:283:GLU:OE1	2.28	0.45
1:E:242:ILE:HD11	1:E:288:ASP:HB3	1.99	0.44
1:F:48:ARG:HA	1:F:51:GLU:HG2	1.97	0.44
1:C:76:ARG:O	1:C:97:ILE:HD11	2.17	0.44
1:D:21:LEU:HD21	1:D:37:GLN:HG3	1.99	0.44
1:E:231:PHE:HE2	1:E:236:MET:CE	2.30	0.44
1:F:211:ALA:HA	1:F:231:PHE:HB2	1.99	0.44
1:B:210:ALA:HB1	1:B:213:SER:OG	2.16	0.44
1:C:355:PRO:HG2	1:C:387:SER:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ALA:HB1	1:E:277:PRO:HD2	1.99	0.44
1:B:123:ASP:OD2	1:B:175:LYS:NZ	2.35	0.44
1:B:384:HIS:CB	1:E:44:GLU:OE1	2.65	0.44
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.75	0.44
1:B:355:PRO:HG2	1:B:387:SER:HB3	1.99	0.44
1:C:191:ASP:OD1	1:C:194:ALA:HB2	2.17	0.44
1:F:30:LEU:HD13	1:F:405:LEU:HD22	2.00	0.44
1:F:191:ASP:O	1:F:195:ILE:HG12	2.17	0.44
1:C:82:PHE:HZ	1:C:307:MET:CE	2.31	0.44
1:A:322:VAL:HG21	1:A:339:GLY:CA	2.46	0.44
1:D:129:ILE:HD12	1:D:129:ILE:HA	1.79	0.44
1:F:235:ARG:CZ	2:F:501:PLG:H4A2	2.47	0.44
1:B:321:LEU:HA	1:B:402:ILE:HG21	2.00	0.44
1:C:235:ARG:HG3	1:C:235:ARG:HH11	1.83	0.44
1:C:76:ARG:HA	1:C:97:ILE:HD11	2.00	0.44
1:B:408:GLY:O	1:B:412:VAL:HG23	2.18	0.43
1:C:383:LEU:O	1:C:384:HIS:HB2	2.17	0.43
1:E:328:LEU:HD22	1:E:330:PHE:CE2	2.53	0.43
1:C:336:SER:O	1:C:342:HIS:NE2	2.31	0.43
1:A:4:THR:O	1:A:8:GLN:HG3	2.18	0.43
1:A:87:ASP:O	1:A:90:ALA:HA	2.19	0.43
1:D:115:GLY:HA3	1:D:142:ILE:HG12	2.01	0.43
1:C:322:VAL:HG11	1:C:339:GLY:CA	2.48	0.43
1:D:76:ARG:NH2	1:D:283:GLU:OE1	2.32	0.43
1:B:336:SER:O	1:B:342:HIS:NE2	2.42	0.43
1:A:191:ASP:OD2	1:A:194:ALA:CB	2.67	0.43
1:C:113[B]:SER:OG	1:C:255:MET:HB3	2.19	0.43
1:E:139:TRP:HA	1:E:142:ILE:HG22	1.99	0.43
1:D:48:ARG:HG2	1:D:51:GLU:OE1	2.19	0.43
1:E:239:PRO:HG3	1:E:294:ALA:HB3	2.00	0.43
1:A:235:ARG:NH2	2:A:501:PLG:C4A	2.72	0.43
1:B:38:ARG:HB2	1:B:43:ILE:HD11	2.01	0.43
1:F:115:GLY:HA3	1:F:142:ILE:HG12	2.01	0.43
1:A:93:GLU:HB3	1:A:96:GLN:NE2	2.34	0.43
1:C:324:GLN:CG	1:C:406:ILE:HG13	2.42	0.42
1:F:195:ILE:HG22	1:F:206:MET:HE3	1.99	0.42
1:B:33:ALA:H	1:B:392:SER:CB	2.32	0.42
1:B:129:ILE:HD12	1:B:129:ILE:HA	1.71	0.42
1:E:276:ALA:HB1	1:E:277:PRO:CD	2.49	0.42
1:A:18:PHE:HB2	1:A:21:LEU:HD12	2.02	0.42
1:C:411:GLN:O	1:C:415:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ARG:HH21	2:D:501:PLG:HA1	1.85	0.42
1:C:137:ILE:HG22	1:E:260:THR:HB	2.01	0.42
1:A:182:VAL:HA	1:A:188:THR:O	2.19	0.42
1:F:373:HIS:HA	1:F:380:LEU:HD22	2.02	0.42
1:A:402:ILE:O	1:A:406:ILE:HG12	2.20	0.42
1:C:317:LEU:HD11	1:C:397:ASN:O	2.20	0.42
1:E:229:LEU:O	1:E:245:LEU:HD12	2.19	0.42
1:E:355:PRO:HG2	1:E:387:SER:CB	2.50	0.42
1:C:126:VAL:HA	1:C:151:VAL:O	2.20	0.41
1:C:131:GLU:CD	1:C:135:ASN:HD22	2.23	0.41
1:E:322:VAL:HG21	1:E:339:GLY:HA3	2.02	0.41
1:D:336:SER:O	1:D:342:HIS:NE2	2.36	0.41
1:A:325:LEU:HD22	1:A:331:VAL:HG11	2.01	0.41
1:C:235:ARG:CZ	2:C:501:PLG:H4A2	2.50	0.41
1:E:76:ARG:HB3	1:E:94:SER:HB2	2.02	0.41
1:E:99:PHE:CZ	1:E:292:ILE:HG23	2.55	0.41
1:E:317:LEU:HD23	1:E:317:LEU:HA	1.77	0.41
1:C:87:ASP:N	1:C:91:LYS:O	2.43	0.41
1:C:322:VAL:HG23	1:C:333:ILE:HD13	2.01	0.41
1:C:338:LEU:O	1:C:341:ASN:HB2	2.20	0.41
1:D:131:GLU:CD	1:D:135:ASN:HD22	2.24	0.41
1:B:98:ILE:HD13	1:B:282:PHE:CD1	2.56	0.41
1:C:153:LEU:HD23	1:C:169:LYS:HB2	2.02	0.41
1:D:132:HIS:CE1	1:D:134:SER:H	2.39	0.41
1:F:362:LEU:HD23	1:F:362:LEU:HA	1.83	0.41
1:A:354:HIS:ND1	1:A:355:PRO:HD2	2.36	0.41
1:B:1:MET:H3	1:B:319:ARG:HH22	1.68	0.41
1:C:180:THR:HA	1:C:209:ASP:HB3	2.03	0.41
1:E:82:PHE:HZ	1:E:307:MET:SD	2.44	0.41
1:E:252:LEU:HD23	1:E:252:LEU:HA	1.83	0.41
1:A:129:ILE:O	1:A:129:ILE:HG13	2.21	0.41
1:B:97:ILE:HG21	1:B:97:ILE:HD13	1.89	0.41
1:B:299:ILE:HD13	1:B:299:ILE:HA	1.80	0.41
1:B:355:PRO:HG2	1:B:387:SER:CB	2.51	0.41
2:B:501:PLG:N	2:B:501:PLG:O3	2.53	0.41
1:E:110:VAL:HG13	1:E:228:LEU:HD13	2.03	0.41
1:E:251:LEU:O	1:E:255:MET:HG3	2.20	0.41
1:B:128:SER:O	1:B:131:GLU:HG2	2.21	0.40
1:C:317:LEU:HA	1:C:317:LEU:HD23	1.74	0.40
1:D:232:SER:HB3	1:D:234:HIS:CD2	2.56	0.40
1:E:195:ILE:H	1:E:195:ILE:HG13	1.71	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HG23	1:A:21:LEU:N	2.36	0.40
1:F:210:ALA:HB1	1:F:213:SER:OG	2.22	0.40
1:A:260:THR:HA	1:A:264:MET:CE	2.51	0.40
1:E:106:ALA:O	1:E:110:VAL:HG23	2.21	0.40
1:C:276:ALA:HB1	1:C:277:PRO:HD2	2.03	0.40
1:C:362:LEU:HD23	1:C:362:LEU:HA	1.93	0.40
1:D:153:LEU:HD23	1:D:169:LYS:HB2	2.03	0.40
1:F:48:ARG:HA	1:F:51:GLU:CG	2.51	0.40
1:C:76:ARG:NH2	1:C:283:GLU:OE1	2.46	0.40
1:D:322:VAL:HG23	1:D:333:ILE:HD13	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	386/447 (86%)	362 (94%)	22 (6%)	2 (0%)	29	68
1	B	388/447 (87%)	375 (97%)	13 (3%)	0	100	100
1	C	387/447 (87%)	376 (97%)	10 (3%)	1 (0%)	41	76
1	D	393/447 (88%)	377 (96%)	16 (4%)	0	100	100
1	E	389/447 (87%)	375 (96%)	14 (4%)	0	100	100
1	F	391/447 (88%)	377 (96%)	11 (3%)	3 (1%)	19	57
All	All	2334/2682 (87%)	2242 (96%)	86 (4%)	6 (0%)	41	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	65	SER
1	F	54	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	263	GLU
1	F	306	ASP
1	A	306	ASP
1	C	306	ASP

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	236/367 (64%)	234 (99%)	2 (1%)	81	93
1	B	246/367 (67%)	246 (100%)	0	100	100
1	C	245/367 (67%)	242 (99%)	3 (1%)	71	90
1	D	254/367 (69%)	250 (98%)	4 (2%)	62	86
1	E	251/367 (68%)	249 (99%)	2 (1%)	81	93
1	F	246/367 (67%)	246 (100%)	0	100	100
All	All	1478/2202 (67%)	1467 (99%)	11 (1%)	91	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113[A]	SER
1	A	113[B]	SER
1	C	113[A]	SER
1	C	113[B]	SER
1	C	384	HIS
1	D	113[A]	SER
1	D	113[B]	SER
1	D	168[A]	SER
1	D	168[B]	SER
1	E	113[A]	SER
1	E	113[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	200	HIS
1	B	24	ASN
1	B	287	GLN
1	C	95	GLN
1	C	140	GLN
1	C	341	ASN
1	D	37	GLN
1	D	200	HIS
1	D	212	GLN
1	D	365	ASN
1	D	404	GLN
1	F	200	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLG	B	501	-	17,20,20	4.23	9 (52%)	23,28,28	1.96	7 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLG	C	501	-	17,20,20	4.22	9 (52%)	23,28,28	1.78	6 (26%)
2	PLG	A	501	-	17,20,20	4.36	8 (47%)	23,28,28	1.60	6 (26%)
2	PLG	F	501	-	17,20,20	4.31	8 (47%)	23,28,28	1.66	3 (13%)
2	PLG	E	501	-	17,20,20	4.30	8 (47%)	23,28,28	1.89	8 (34%)
2	PLG	D	501	-	17,20,20	4.44	10 (58%)	23,28,28	1.81	9 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	B	501	-	-	3/10/12/12	0/1/1/1
2	PLG	C	501	-	-	3/10/12/12	0/1/1/1
2	PLG	A	501	-	-	3/10/12/12	0/1/1/1
2	PLG	F	501	-	-	3/10/12/12	0/1/1/1
2	PLG	E	501	-	-	3/10/12/12	0/1/1/1
2	PLG	D	501	-	-	3/10/12/12	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLG	C3-C2	-9.16	1.31	1.40
2	E	501	PLG	C3-C2	-8.98	1.31	1.40
2	D	501	PLG	C3-C2	-8.87	1.32	1.40
2	F	501	PLG	C3-C2	-8.76	1.32	1.40
2	C	501	PLG	C2-N1	8.62	1.50	1.33
2	D	501	PLG	C2-N1	8.40	1.49	1.33
2	B	501	PLG	C3-C2	-8.38	1.32	1.40
2	B	501	PLG	C5-C4	-8.33	1.28	1.40
2	E	501	PLG	C5-C4	-8.26	1.28	1.40
2	B	501	PLG	C2-N1	8.09	1.49	1.33
2	A	501	PLG	C5-C4	-8.01	1.29	1.40
2	F	501	PLG	C2-N1	8.00	1.48	1.33
2	C	501	PLG	C3-C2	-7.97	1.32	1.40
2	F	501	PLG	C5-C4	-7.92	1.29	1.40
2	D	501	PLG	C5-C4	-7.87	1.29	1.40
2	A	501	PLG	C2-N1	7.85	1.48	1.33
2	E	501	PLG	C2-N1	7.73	1.48	1.33
2	C	501	PLG	C5-C4	-6.98	1.30	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLG	C6-C5	6.70	1.51	1.37
2	D	501	PLG	C3-C4	6.65	1.50	1.40
2	F	501	PLG	C6-C5	6.61	1.51	1.37
2	D	501	PLG	C6-C5	6.50	1.51	1.37
2	A	501	PLG	C6-C5	6.46	1.51	1.37
2	A	501	PLG	C3-C4	6.44	1.49	1.40
2	B	501	PLG	C6-C5	6.27	1.50	1.37
2	E	501	PLG	C6-C5	6.22	1.50	1.37
2	C	501	PLG	C3-C4	6.09	1.49	1.40
2	F	501	PLG	C3-C4	5.85	1.49	1.40
2	E	501	PLG	C3-C4	5.70	1.48	1.40
2	B	501	PLG	C3-C4	5.38	1.48	1.40
2	E	501	PLG	C6-N1	-3.36	1.27	1.34
2	F	501	PLG	C6-N1	-3.30	1.27	1.34
2	D	501	PLG	C6-N1	-3.29	1.27	1.34
2	C	501	PLG	C6-N1	-3.16	1.27	1.34
2	A	501	PLG	C6-N1	-3.16	1.27	1.34
2	B	501	PLG	C6-N1	-3.08	1.27	1.34
2	D	501	PLG	P-OP3	-2.90	1.43	1.54
2	F	501	PLG	P-OP2	-2.68	1.44	1.54
2	C	501	PLG	P-OP2	-2.63	1.44	1.54
2	A	501	PLG	P-OP2	-2.44	1.45	1.54
2	E	501	PLG	P-OP3	-2.34	1.45	1.54
2	D	501	PLG	C2A-C2	2.33	1.54	1.50
2	F	501	PLG	P-OP3	-2.33	1.45	1.54
2	E	501	PLG	P-OP1	-2.28	1.43	1.50
2	C	501	PLG	P-OP3	-2.21	1.46	1.54
2	B	501	PLG	P-OP2	-2.21	1.46	1.54
2	D	501	PLG	P-OP2	-2.15	1.46	1.54
2	B	501	PLG	P-OP1	-2.14	1.43	1.50
2	D	501	PLG	P-OP4	2.12	1.67	1.60
2	C	501	PLG	C2A-C2	2.11	1.54	1.50
2	A	501	PLG	P-OP4	2.09	1.66	1.60
2	B	501	PLG	P-OP3	-2.06	1.46	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLG	OP3-P-OP4	5.22	120.61	106.73
2	C	501	PLG	OP4-P-OP1	4.81	119.98	106.47
2	E	501	PLG	OP2-P-OP4	4.51	118.74	106.73
2	D	501	PLG	OP4-P-OP1	4.50	119.08	106.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	PLG	OP4-P-OP1	4.28	118.49	106.47
2	F	501	PLG	C6-C5-C4	3.92	120.89	118.12
2	A	501	PLG	OP4-P-OP1	3.70	116.86	106.47
2	A	501	PLG	C3-C4-C5	3.02	121.62	118.72
2	D	501	PLG	OP3-P-OP1	-2.97	99.06	110.68
2	F	501	PLG	C5-C6-N1	-2.68	119.35	123.82
2	C	501	PLG	C5-C6-N1	-2.64	119.42	123.82
2	B	501	PLG	C4A-C4-C3	-2.63	117.23	120.04
2	E	501	PLG	C5-C6-N1	-2.58	119.52	123.82
2	B	501	PLG	OP3-P-OP1	-2.58	100.58	110.68
2	B	501	PLG	C5-C6-N1	-2.58	119.53	123.82
2	B	501	PLG	O3-C3-C2	2.57	123.09	117.49
2	E	501	PLG	C3-C4-C5	2.54	121.16	118.72
2	C	501	PLG	C3-C4-C5	2.54	121.16	118.72
2	C	501	PLG	C-CA-N	-2.53	106.27	111.43
2	E	501	PLG	O3-C3-C2	2.49	122.92	117.49
2	B	501	PLG	C3-C4-C5	2.47	121.09	118.72
2	E	501	PLG	OP3-P-OP4	2.46	113.27	106.73
2	D	501	PLG	C3-C4-C5	2.38	121.00	118.72
2	A	501	PLG	C5-C6-N1	-2.37	119.88	123.82
2	E	501	PLG	C4A-C4-C3	-2.33	117.55	120.04
2	D	501	PLG	OP2-P-OP4	2.29	112.82	106.73
2	E	501	PLG	CA-N-C4A	-2.29	106.78	112.54
2	C	501	PLG	OP2-P-OP1	-2.28	101.74	110.68
2	B	501	PLG	C4-C4A-N	2.28	115.84	111.58
2	D	501	PLG	OP3-P-OP4	2.28	112.80	106.73
2	E	501	PLG	OP2-P-OP1	-2.25	101.87	110.68
2	D	501	PLG	C5-C6-N1	-2.15	120.23	123.82
2	A	501	PLG	OP2-P-OP1	-2.15	102.27	110.68
2	A	501	PLG	C4A-C4-C3	-2.06	117.84	120.04
2	D	501	PLG	C-CA-N	2.05	115.63	111.43
2	C	501	PLG	O3-C3-C2	2.03	121.92	117.49
2	A	501	PLG	OP3-P-OP4	2.03	112.13	106.73
2	D	501	PLG	C3-C2-N1	-2.02	118.16	120.77
2	D	501	PLG	C2A-C2-N1	2.01	121.59	117.67

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLG	C5-C4-C4A-N
2	B	501	PLG	C5-C4-C4A-N

Continued on next page...

Continued from previous page...

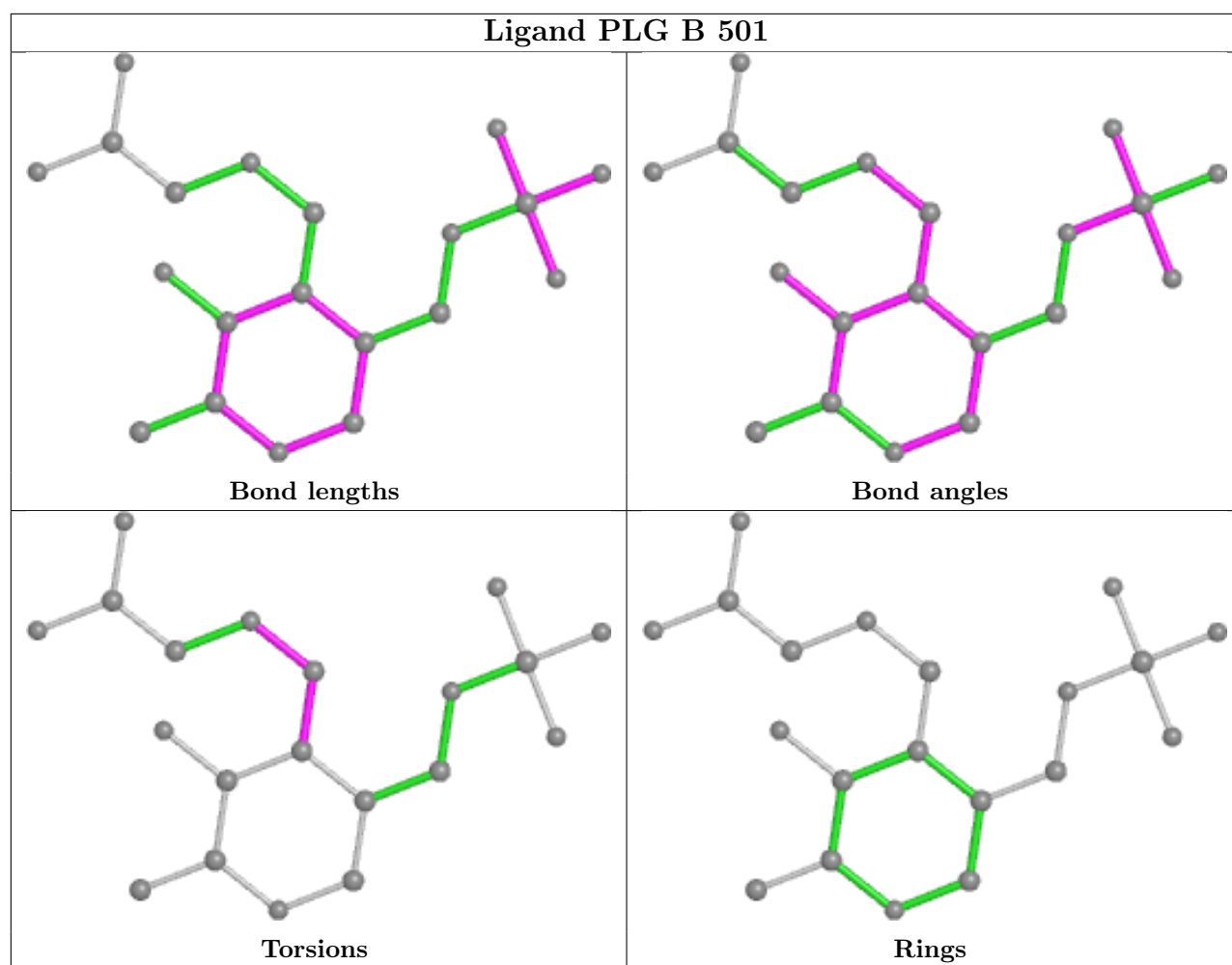
Mol	Chain	Res	Type	Atoms
2	C	501	PLG	C5-C4-C4A-N
2	D	501	PLG	C5-C4-C4A-N
2	E	501	PLG	C5-C4-C4A-N
2	F	501	PLG	C5-C4-C4A-N
2	A	501	PLG	C3-C4-C4A-N
2	A	501	PLG	C5A-OP4-P-OP1
2	D	501	PLG	C4-C4A-N-CA
2	B	501	PLG	C3-C4-C4A-N
2	C	501	PLG	C3-C4-C4A-N
2	D	501	PLG	C3-C4-C4A-N
2	E	501	PLG	C3-C4-C4A-N
2	F	501	PLG	C3-C4-C4A-N
2	B	501	PLG	C4-C4A-N-CA
2	C	501	PLG	C4-C4A-N-CA
2	E	501	PLG	C4-C4A-N-CA
2	F	501	PLG	C4-C4A-N-CA

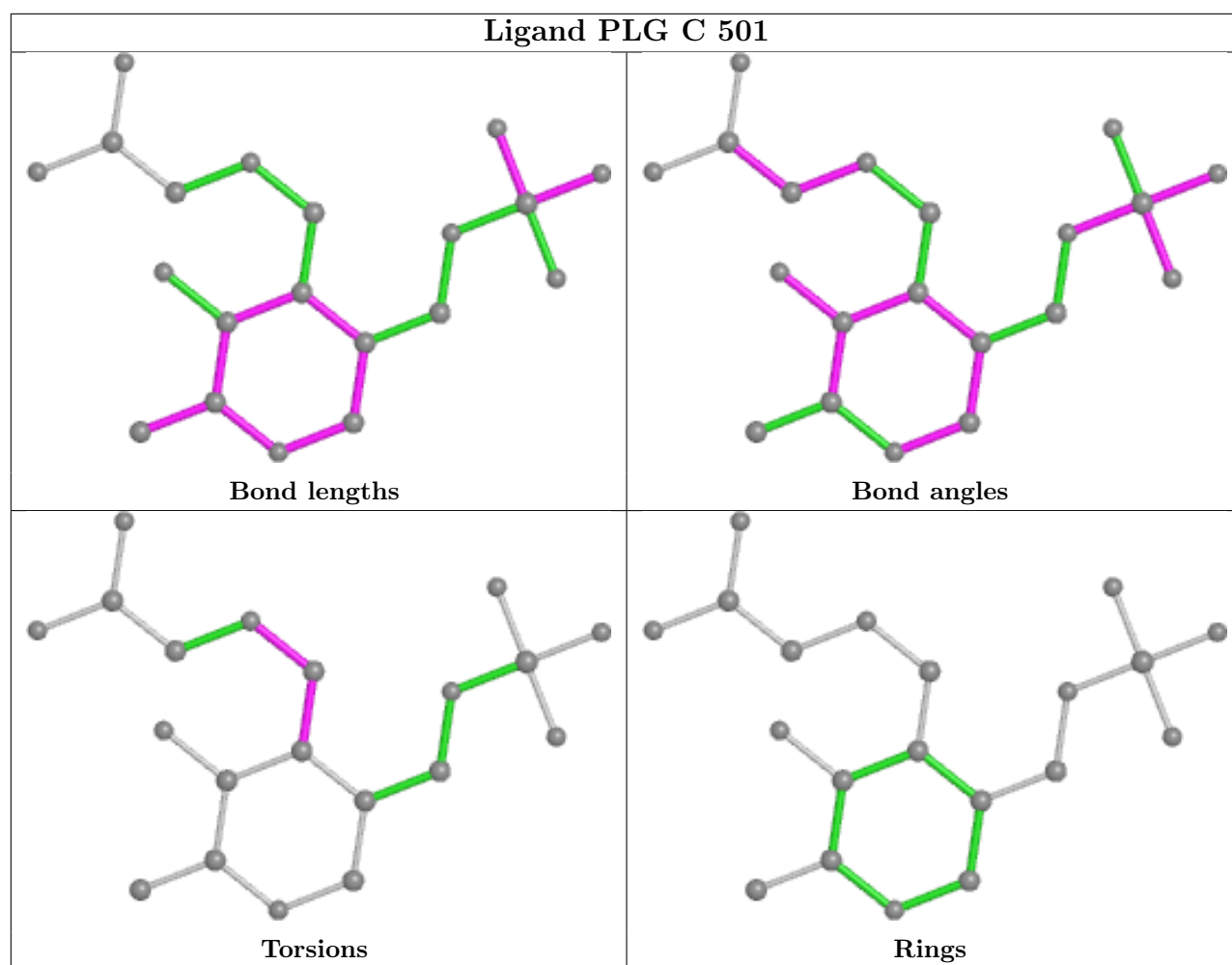
There are no ring outliers.

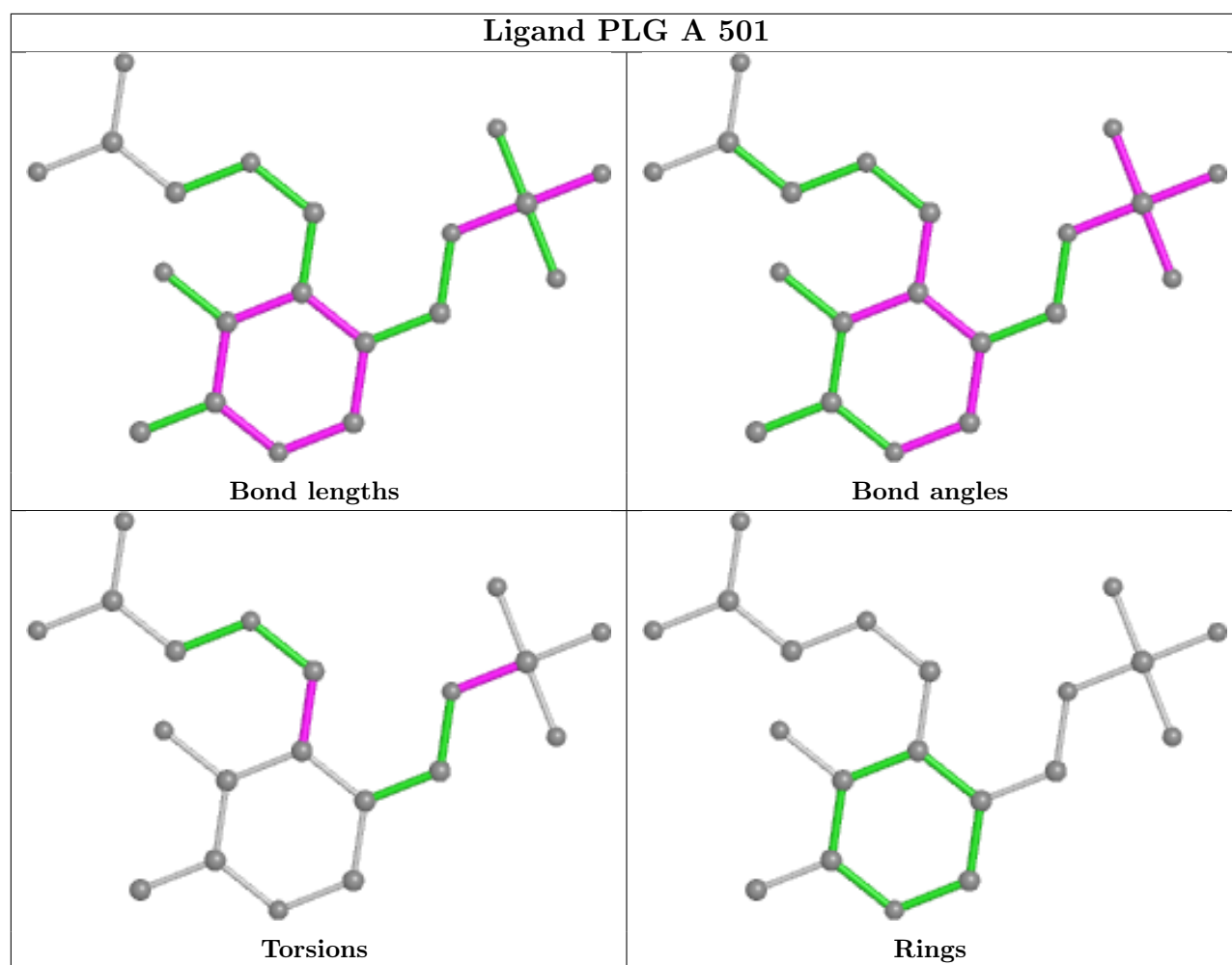
6 monomers are involved in 25 short contacts:

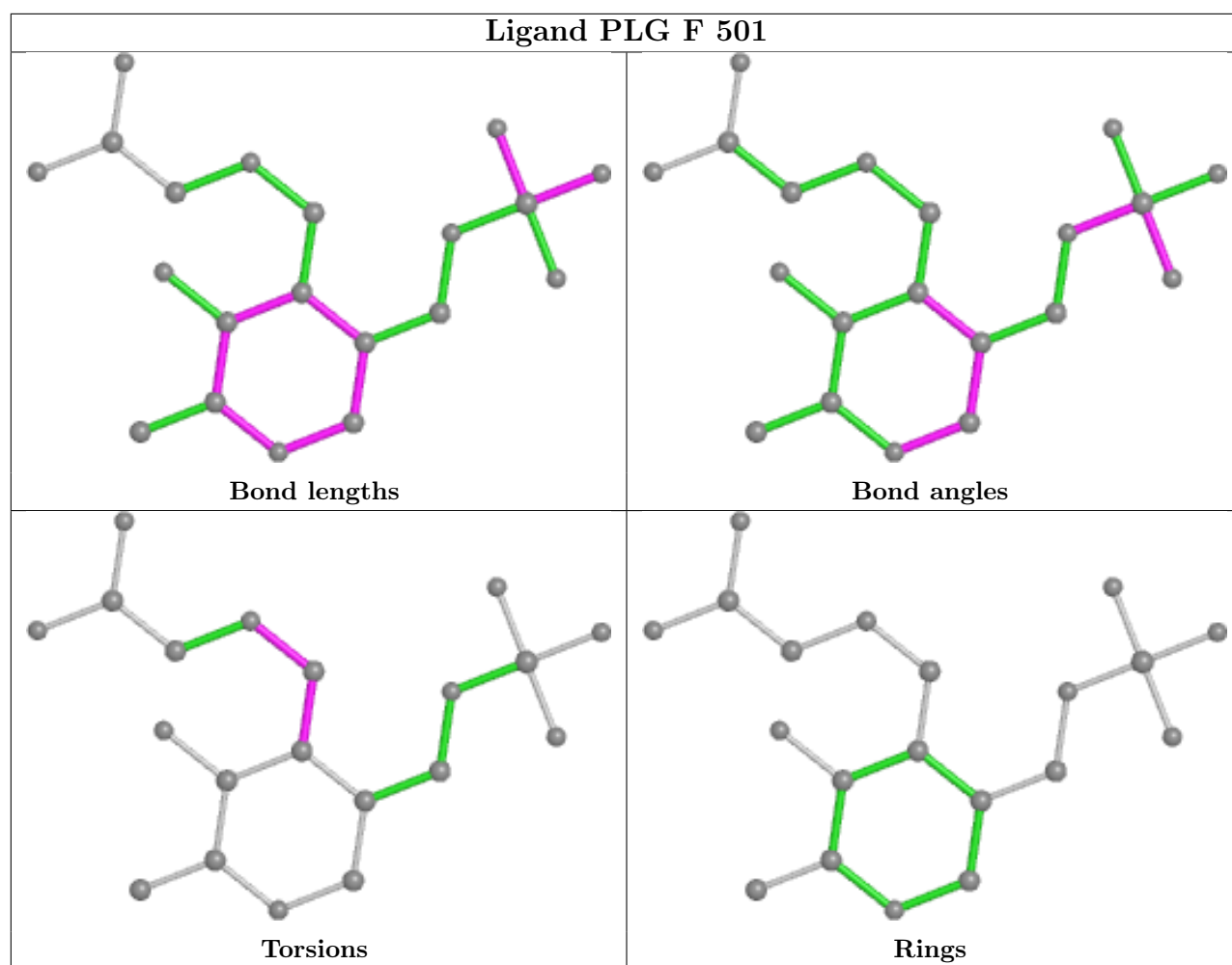
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PLG	4	0
2	C	501	PLG	3	0
2	A	501	PLG	7	0
2	F	501	PLG	3	0
2	E	501	PLG	4	0
2	D	501	PLG	4	0

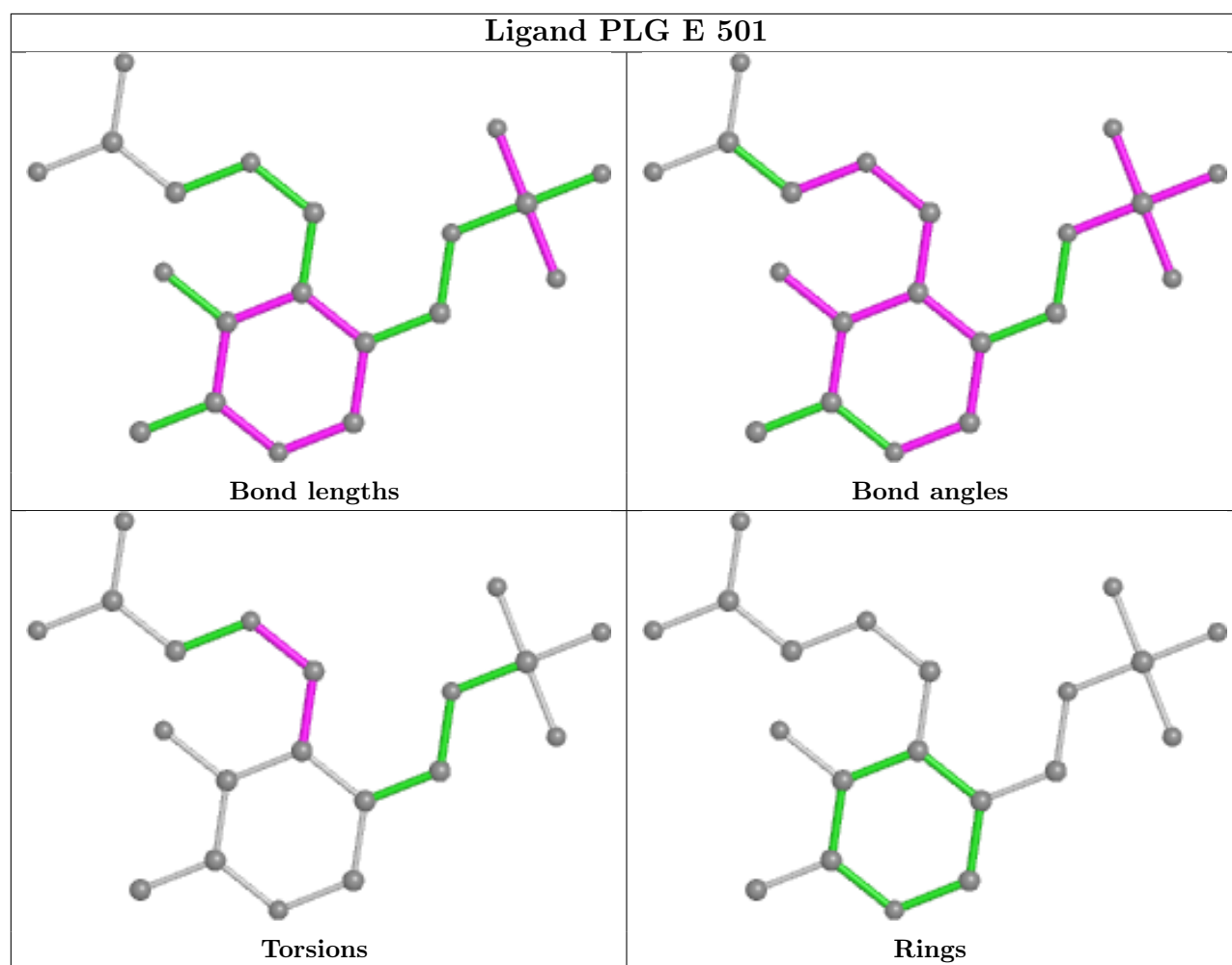
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

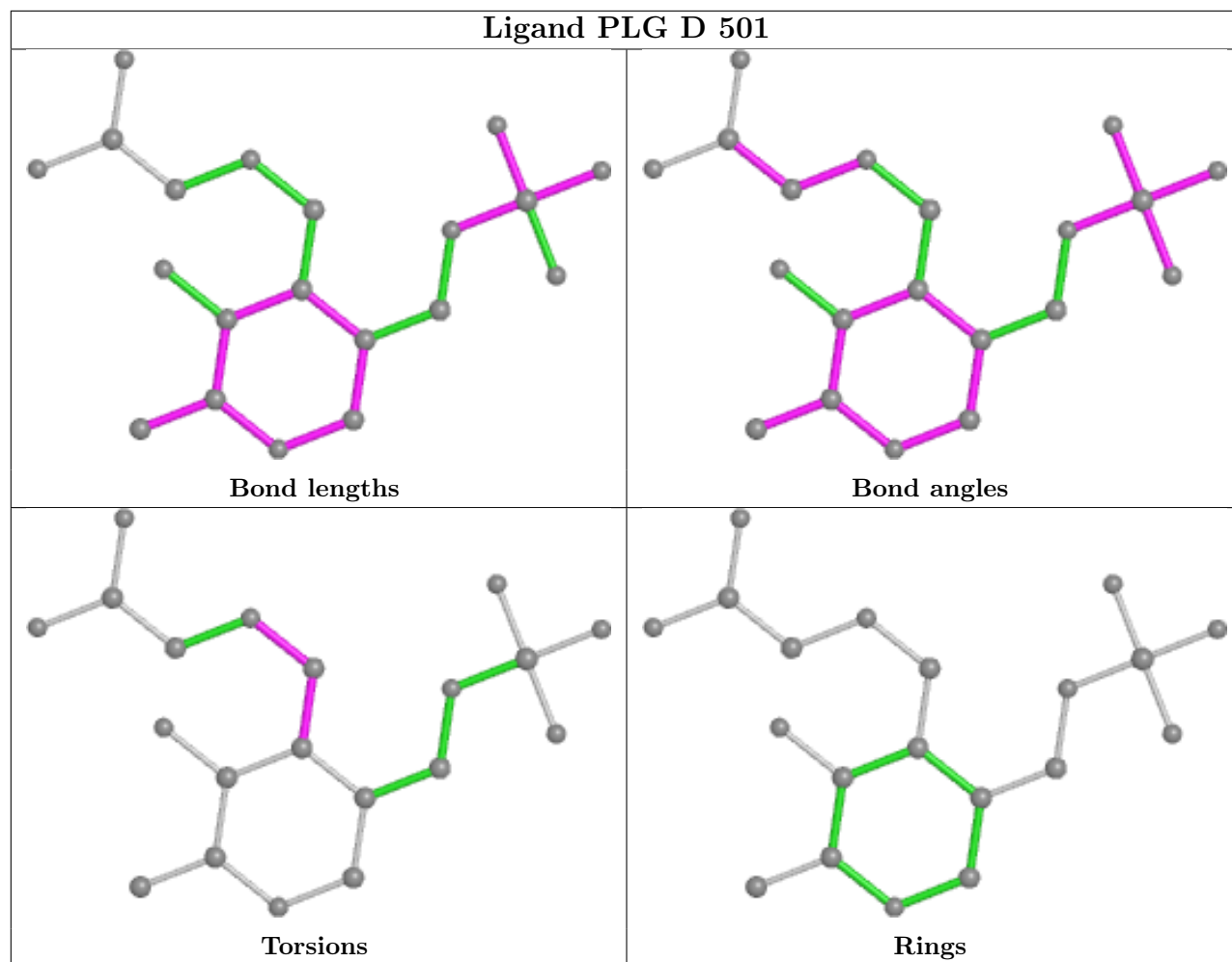












5.7 Other polymers [i](#)

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	391/447 (87%)	0.53	21 (5%)	25 9	50, 59, 73, 96	0
1	B	393/447 (87%)	0.52	24 (6%)	21 7	50, 58, 77, 101	0
1	C	392/447 (87%)	0.63	39 (9%)	7 2	52, 61, 78, 104	0
1	D	398/447 (89%)	0.62	34 (8%)	10 3	51, 61, 78, 92	0
1	E	395/447 (88%)	0.64	42 (10%)	6 2	51, 60, 74, 93	0
1	F	396/447 (88%)	0.73	47 (11%)	4 1	52, 61, 80, 118	0
All	All	2365/2682 (88%)	0.61	207 (8%)	10 3	50, 60, 77, 118	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	28	ALA	7.2
1	D	55	ALA	6.4
1	D	22	ALA	5.8
1	E	28	ALA	5.6
1	D	374	HIS	5.2
1	B	282	PHE	5.2
1	F	298	ALA	5.1
1	F	75	ALA	4.7
1	E	178	SER	4.6
1	F	153	LEU	4.4
1	C	26	LYS	4.3
1	E	20	ILE	4.3
1	C	324	GLN	4.2
1	C	282	PHE	4.1
1	C	55	ALA	4.0
1	F	23	ALA	4.0
1	F	190	ASN	4.0
1	B	402	ILE	4.0
1	E	24	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	54	ASN	3.9
1	A	332	ASP	3.8
1	C	208	VAL	3.8
1	C	23	ALA	3.8
1	C	174	ALA	3.8
1	A	353	VAL	3.7
1	D	275	TRP	3.7
1	F	246	TRP	3.7
1	F	64	TRP	3.7
1	E	374	HIS	3.7
1	F	284	ALA	3.7
1	F	244	VAL	3.6
1	A	244	VAL	3.6
1	C	345	ALA	3.6
1	A	388	THR	3.5
1	C	229	LEU	3.5
1	E	179	VAL	3.5
1	C	119	LEU	3.4
1	D	327	THR	3.4
1	D	64	TRP	3.4
1	D	219	VAL	3.4
1	A	251	LEU	3.3
1	B	378	PRO	3.3
1	D	179	VAL	3.3
1	C	257	PRO	3.3
1	E	22	ALA	3.3
1	C	352	GLY	3.3
1	F	70	ALA	3.3
1	F	243	GLY	3.1
1	B	117	TYR	3.1
1	E	180	THR	3.1
1	E	295	THR	3.1
1	C	375	CYS	3.1
1	D	180	THR	3.1
1	A	53	MET	3.0
1	E	233	ALA	3.0
1	C	209	ASP	3.0
1	B	208	VAL	3.0
1	C	34	ALA	3.0
1	C	330	PHE	3.0
1	F	34	ALA	2.9
1	D	234	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	52	THR	2.9
1	E	336	SER	2.9
1	E	387	SER	2.9
1	F	299	ILE	2.9
1	F	239	PRO	2.8
1	E	177	VAL	2.8
1	D	205	TYR	2.8
1	E	212	GLN	2.8
1	D	276	ALA	2.8
1	D	151	VAL	2.8
1	C	212	GLN	2.8
1	B	222	HIS	2.8
1	F	302	LEU	2.8
1	C	204	ALA	2.8
1	F	343	VAL	2.7
1	D	123	ASP	2.7
1	F	43	ILE	2.7
1	F	183	SER	2.7
1	B	28	ALA	2.7
1	A	302	LEU	2.7
1	C	113[A]	SER	2.7
1	F	310	ILE	2.7
1	D	301	TYR	2.7
1	D	53	MET	2.6
1	E	405	LEU	2.6
1	F	98	ILE	2.6
1	F	346	VAL	2.6
1	C	52	THR	2.6
1	C	402	ILE	2.6
1	C	159	TYR	2.6
1	E	163	PRO	2.6
1	E	255	MET	2.6
1	A	375	CYS	2.6
1	A	243	GLY	2.6
1	C	231	PHE	2.6
1	D	231	PHE	2.6
1	E	176	ILE	2.6
1	C	353	VAL	2.6
1	E	282	PHE	2.5
1	F	256	PRO	2.5
1	F	229	LEU	2.5
1	B	99	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	332	ASP	2.5
1	E	388	THR	2.5
1	B	371	ALA	2.5
1	C	178	SER	2.5
1	B	22	ALA	2.4
1	E	46	GLN	2.4
1	A	176	ILE	2.4
1	C	320	TYR	2.4
1	C	368[A]	CYS	2.4
1	F	121	PRO	2.4
1	D	353	VAL	2.4
1	E	288	ASP	2.4
1	D	167	ALA	2.4
1	D	239	PRO	2.4
1	E	254	ALA	2.4
1	E	393	VAL	2.4
1	E	296	GLY	2.4
1	B	174	ALA	2.4
1	A	98	ILE	2.4
1	D	282	PHE	2.4
1	A	298	ALA	2.4
1	F	218	LEU	2.4
1	F	393	VAL	2.4
1	A	113[A]	SER	2.4
1	E	99	PHE	2.3
1	F	282	PHE	2.3
1	B	387	SER	2.3
1	C	117	TYR	2.3
1	B	21	LEU	2.3
1	E	187	GLY	2.3
1	C	177	VAL	2.3
1	C	278	VAL	2.3
1	D	46	GLN	2.3
1	B	119	LEU	2.3
1	F	65	SER	2.3
1	C	413	TRP	2.3
1	C	376	ALA	2.3
1	E	55	ALA	2.3
1	E	410	ASN	2.3
1	C	67	ASP	2.3
1	E	337	LYS	2.3
1	F	55	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	244	VAL	2.3
1	F	413	TRP	2.3
1	B	23	ALA	2.3
1	E	239	PRO	2.3
1	A	348	PHE	2.3
1	D	287	GLN	2.3
1	E	54	ASN	2.3
1	F	184	ASN	2.2
1	A	211	ALA	2.2
1	F	416	PHE	2.2
1	B	380	LEU	2.2
1	E	204	ALA	2.2
1	F	347	ALA	2.2
1	D	149	ASN	2.2
1	C	30	LEU	2.2
1	E	117	TYR	2.2
1	F	388	THR	2.2
1	D	196	ALA	2.2
1	D	375	CYS	2.2
1	D	367	VAL	2.2
1	F	135	ASN	2.2
1	C	75	ALA	2.2
1	F	79	ILE	2.2
1	E	219	VAL	2.2
1	B	239	PRO	2.2
1	B	207	VAL	2.2
1	A	371	ALA	2.2
1	D	368	CYS	2.2
1	B	290	ALA	2.2
1	C	297	ALA	2.1
1	C	256	PRO	2.1
1	F	334	VAL	2.1
1	F	191	ASP	2.1
1	B	214	ALA	2.1
1	E	214	ALA	2.1
1	F	196	ALA	2.1
1	F	178	SER	2.1
1	C	328	LEU	2.1
1	B	347	ALA	2.1
1	F	206	MET	2.1
1	F	296	GLY	2.1
1	B	348	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	401	ASP	2.1
1	F	404	GLN	2.1
1	A	256	PRO	2.1
1	F	328	LEU	2.1
1	E	401	ASP	2.1
1	E	366	ASN	2.1
1	D	182	VAL	2.1
1	A	14	TYR	2.1
1	D	104	SER	2.1
1	A	191	ASP	2.1
1	E	124	ASP	2.1
1	B	52	THR	2.1
1	A	123	ASP	2.0
1	F	209	ASP	2.0
1	B	1	MET	2.0
1	D	126	VAL	2.0
1	E	397	ASN	2.0
1	E	235	ARG	2.0
1	E	392	SER	2.0
1	F	231	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLG	C	501	20/20	0.89	0.24	54,56,58,60	0
2	PLG	E	501	20/20	0.91	0.21	54,55,57,57	0
2	PLG	F	501	20/20	0.92	0.22	55,57,60,62	0

Continued on next page...

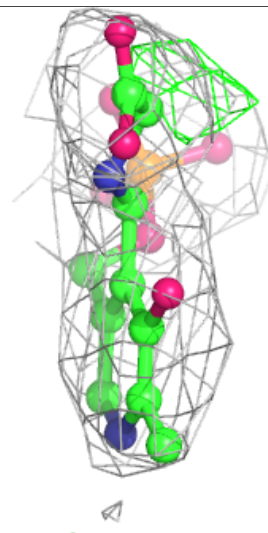
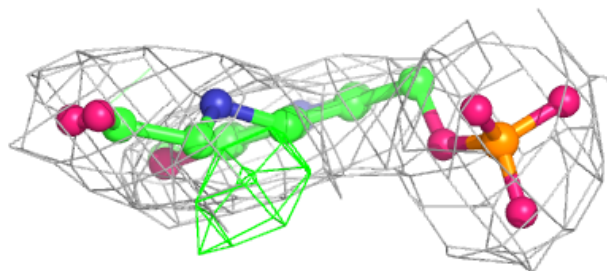
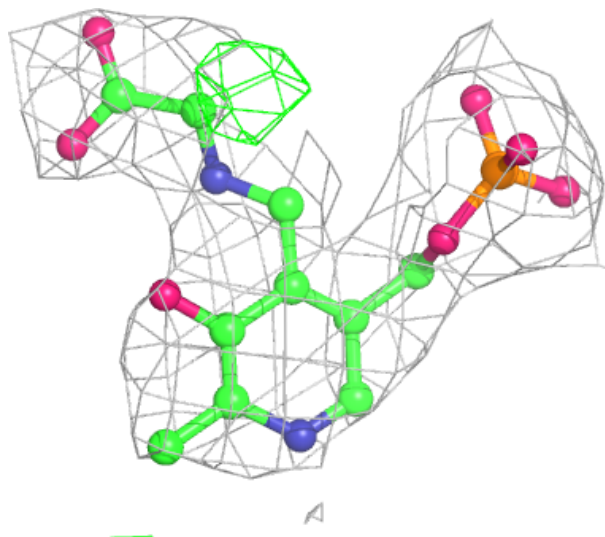
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PLG	B	501	20/20	0.93	0.26	50,53,54,54	0
2	PLG	A	501	20/20	0.93	0.22	51,53,54,56	0
2	PLG	D	501	20/20	0.94	0.19	53,54,55,56	0

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

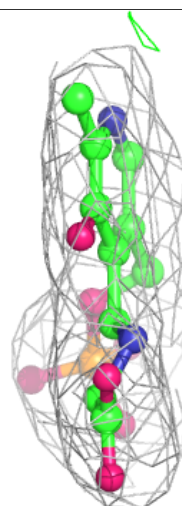
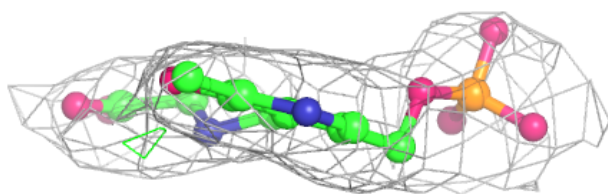
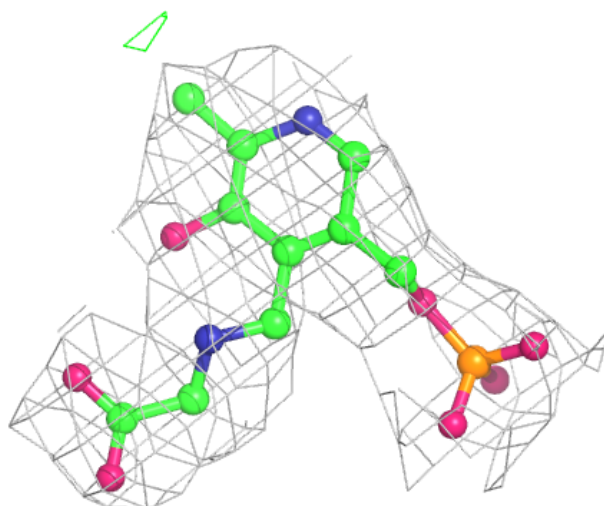
Electron density around PLG C 501:

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



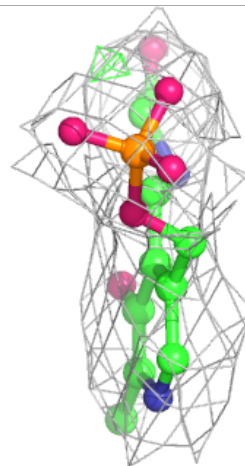
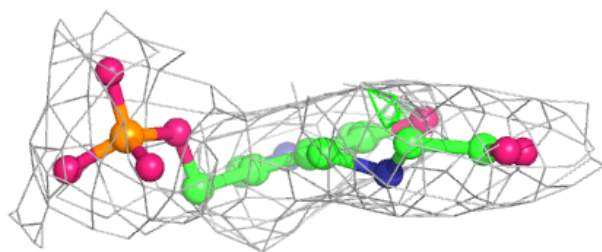
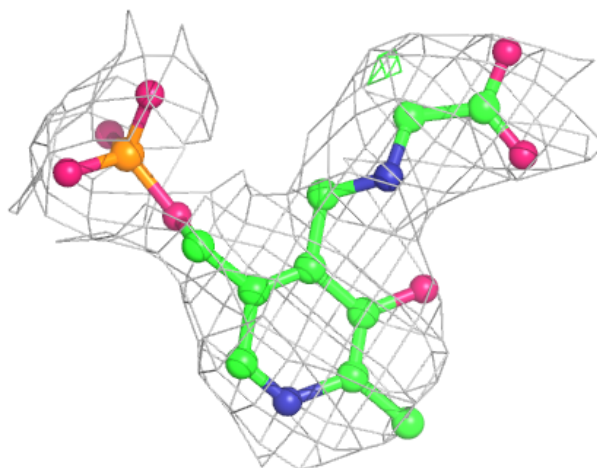
Electron density around PLG E 501:

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



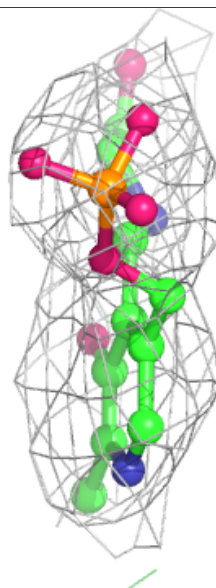
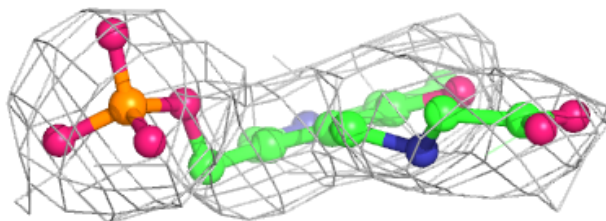
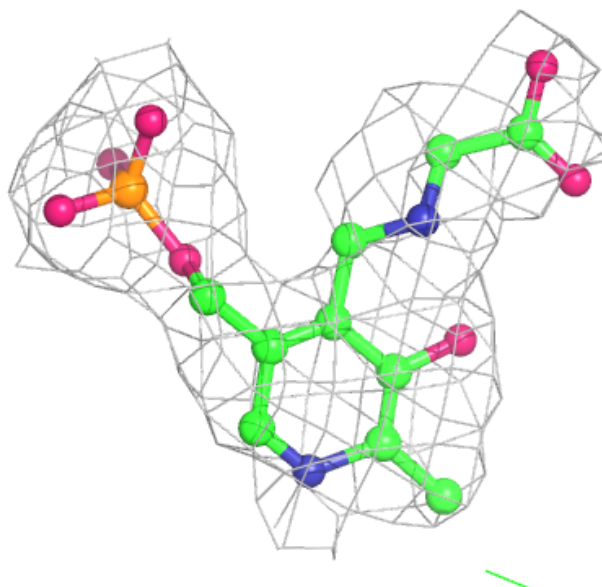
Electron density around PLG F 501:

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



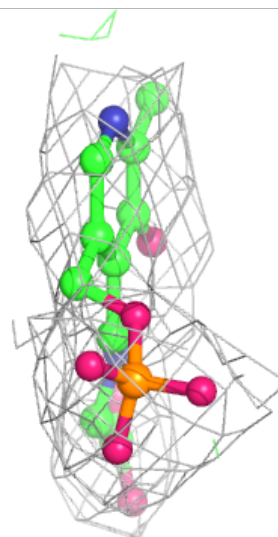
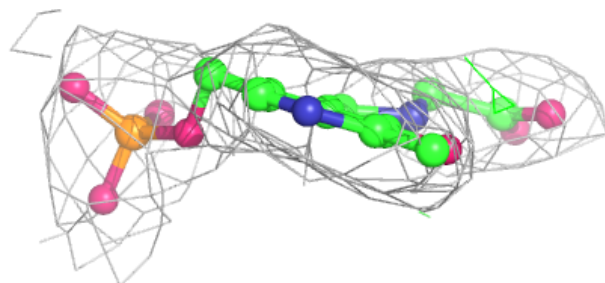
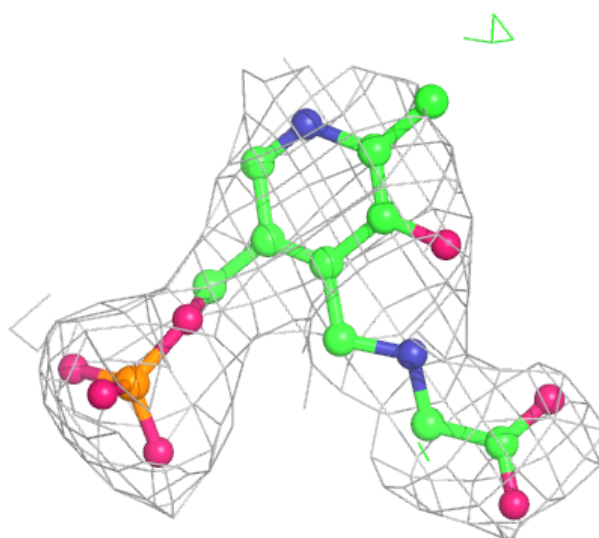
Electron density around PLG B 501:

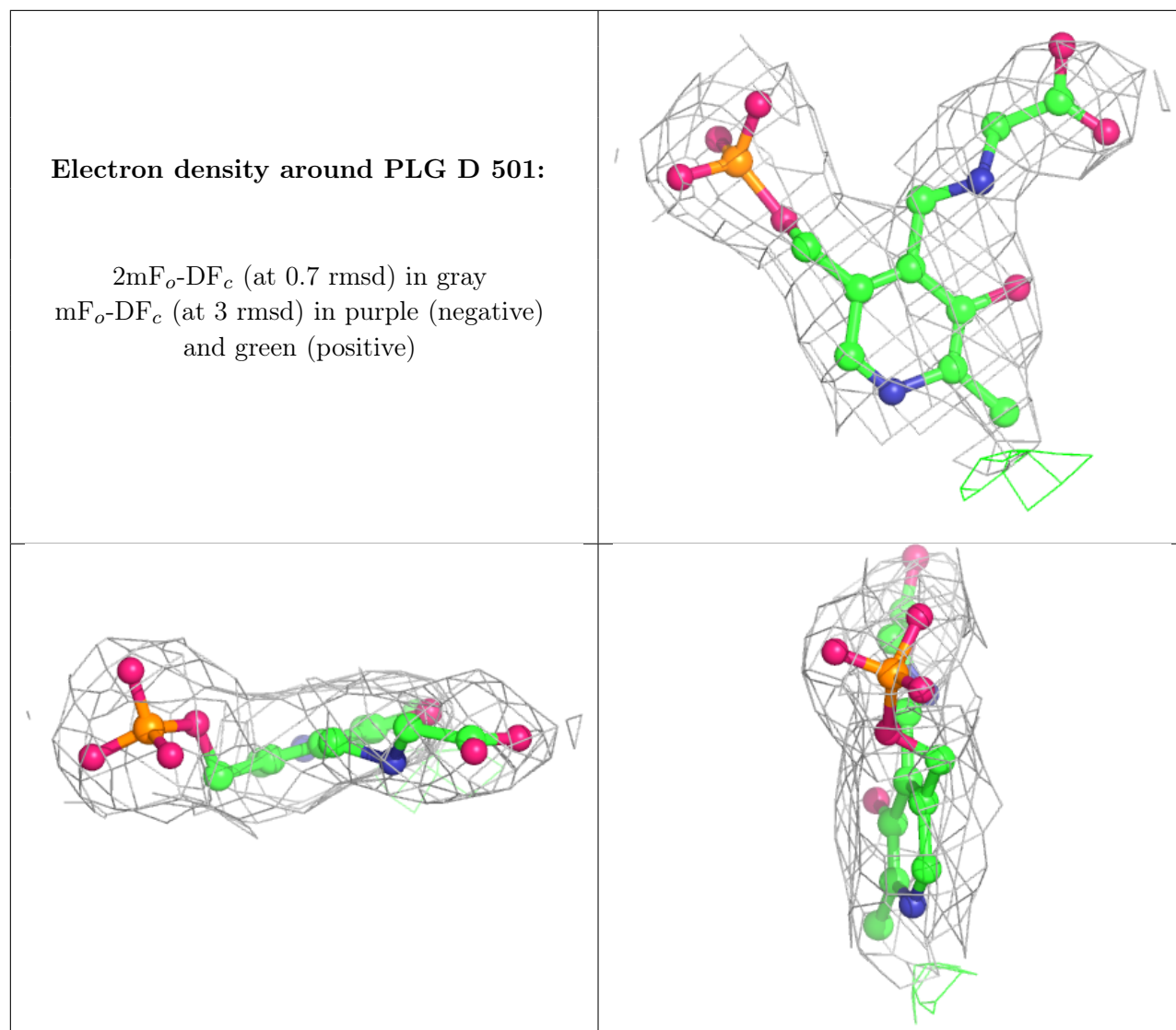
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLG A 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.