



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:11 PM BST

PDB ID : 5TSU  
Title : Active conformation for Engineered human cystathionine gamma lyase (E59N, R119L, E339V) to depleting methionine  
Authors : Yan, W.; Zhang, Y.  
Deposited on : 2016-10-31  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
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) : 2.14.4.dev1

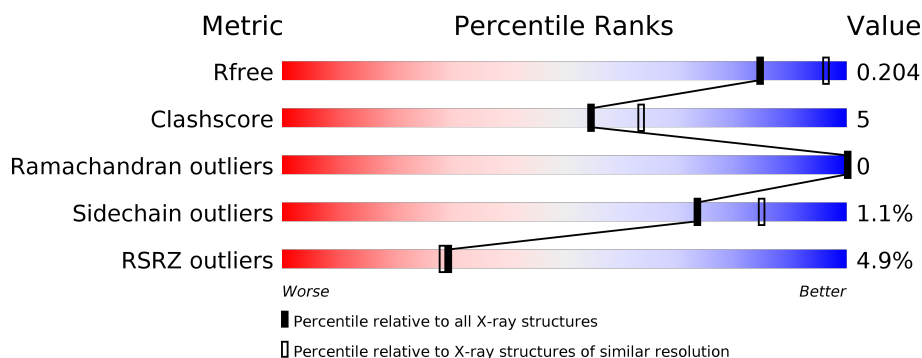
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	B	422	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	D	422	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>9%</div> </div> </div>
1	F	422	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
1	G	422	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>
1	H	422	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	422	<div><div><div>2%</div><div>81%</div><div>10%</div><div>9%</div></div></div>
2	E	422	<div><div><div>2%</div><div>80%</div><div>11%</div><div>9%</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24978 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 Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	P	S	0	0	0
			2985	1905	507	553	1	19			
1	B	385	Total	C	N	O	P	S	0	0	0
			2992	1909	508	555	1	19			
1	D	384	Total	C	N	O	P	S	0	0	0
			2976	1898	505	553	1	19			
1	F	381	Total	C	N	O	P	S	0	0	0
			2961	1889	503	549	1	19			
1	G	386	Total	C	N	O	P	S	0	0	0
			2996	1913	508	555	1	19			
1	H	386	Total	C	N	O	P	S	0	0	0
			3001	1915	509	557	1	19			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP P32929
A	-15	GLY	-	expression tag	UNP P32929
A	-14	GLY	-	expression tag	UNP P32929
A	-13	HIS	-	expression tag	UNP P32929
A	-12	HIS	-	expression tag	UNP P32929
A	-11	HIS	-	expression tag	UNP P32929
A	-10	HIS	-	expression tag	UNP P32929
A	-9	HIS	-	expression tag	UNP P32929
A	-8	HIS	-	expression tag	UNP P32929
A	-7	GLY	-	expression tag	UNP P32929
A	-6	LEU	-	expression tag	UNP P32929
A	-5	GLU	-	expression tag	UNP P32929
A	-4	VAL	-	expression tag	UNP P32929
A	-3	LEU	-	expression tag	UNP P32929
A	-2	PHE	-	expression tag	UNP P32929
A	-1	GLN	-	expression tag	UNP P32929
A	0	GLY	-	expression tag	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP P32929
A	59	ASN	GLU	engineered mutation	UNP P32929
A	119	LEU	ARG	engineered mutation	UNP P32929
A	339	VAL	GLU	engineered mutation	UNP P32929
B	-16	MET	-	expression tag	UNP P32929
B	-15	GLY	-	expression tag	UNP P32929
B	-14	GLY	-	expression tag	UNP P32929
B	-13	HIS	-	expression tag	UNP P32929
B	-12	HIS	-	expression tag	UNP P32929
B	-11	HIS	-	expression tag	UNP P32929
B	-10	HIS	-	expression tag	UNP P32929
B	-9	HIS	-	expression tag	UNP P32929
B	-8	HIS	-	expression tag	UNP P32929
B	-7	GLY	-	expression tag	UNP P32929
B	-6	LEU	-	expression tag	UNP P32929
B	-5	GLU	-	expression tag	UNP P32929
B	-4	VAL	-	expression tag	UNP P32929
B	-3	LEU	-	expression tag	UNP P32929
B	-2	PHE	-	expression tag	UNP P32929
B	-1	GLN	-	expression tag	UNP P32929
B	0	GLY	-	expression tag	UNP P32929
B	1	PRO	-	expression tag	UNP P32929
B	59	ASN	GLU	engineered mutation	UNP P32929
B	119	LEU	ARG	engineered mutation	UNP P32929
B	339	VAL	GLU	engineered mutation	UNP P32929
D	-16	MET	-	expression tag	UNP P32929
D	-15	GLY	-	expression tag	UNP P32929
D	-14	GLY	-	expression tag	UNP P32929
D	-13	HIS	-	expression tag	UNP P32929
D	-12	HIS	-	expression tag	UNP P32929
D	-11	HIS	-	expression tag	UNP P32929
D	-10	HIS	-	expression tag	UNP P32929
D	-9	HIS	-	expression tag	UNP P32929
D	-8	HIS	-	expression tag	UNP P32929
D	-7	GLY	-	expression tag	UNP P32929
D	-6	LEU	-	expression tag	UNP P32929
D	-5	GLU	-	expression tag	UNP P32929
D	-4	VAL	-	expression tag	UNP P32929
D	-3	LEU	-	expression tag	UNP P32929
D	-2	PHE	-	expression tag	UNP P32929
D	-1	GLN	-	expression tag	UNP P32929
D	0	GLY	-	expression tag	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	PRO	-	expression tag	UNP P32929
D	59	ASN	GLU	engineered mutation	UNP P32929
D	119	LEU	ARG	engineered mutation	UNP P32929
D	339	VAL	GLU	engineered mutation	UNP P32929
F	-16	MET	-	expression tag	UNP P32929
F	-15	GLY	-	expression tag	UNP P32929
F	-14	GLY	-	expression tag	UNP P32929
F	-13	HIS	-	expression tag	UNP P32929
F	-12	HIS	-	expression tag	UNP P32929
F	-11	HIS	-	expression tag	UNP P32929
F	-10	HIS	-	expression tag	UNP P32929
F	-9	HIS	-	expression tag	UNP P32929
F	-8	HIS	-	expression tag	UNP P32929
F	-7	GLY	-	expression tag	UNP P32929
F	-6	LEU	-	expression tag	UNP P32929
F	-5	GLU	-	expression tag	UNP P32929
F	-4	VAL	-	expression tag	UNP P32929
F	-3	LEU	-	expression tag	UNP P32929
F	-2	PHE	-	expression tag	UNP P32929
F	-1	GLN	-	expression tag	UNP P32929
F	0	GLY	-	expression tag	UNP P32929
F	1	PRO	-	expression tag	UNP P32929
F	59	ASN	GLU	engineered mutation	UNP P32929
F	119	LEU	ARG	engineered mutation	UNP P32929
F	339	VAL	GLU	engineered mutation	UNP P32929
G	-16	MET	-	expression tag	UNP P32929
G	-15	GLY	-	expression tag	UNP P32929
G	-14	GLY	-	expression tag	UNP P32929
G	-13	HIS	-	expression tag	UNP P32929
G	-12	HIS	-	expression tag	UNP P32929
G	-11	HIS	-	expression tag	UNP P32929
G	-10	HIS	-	expression tag	UNP P32929
G	-9	HIS	-	expression tag	UNP P32929
G	-8	HIS	-	expression tag	UNP P32929
G	-7	GLY	-	expression tag	UNP P32929
G	-6	LEU	-	expression tag	UNP P32929
G	-5	GLU	-	expression tag	UNP P32929
G	-4	VAL	-	expression tag	UNP P32929
G	-3	LEU	-	expression tag	UNP P32929
G	-2	PHE	-	expression tag	UNP P32929
G	-1	GLN	-	expression tag	UNP P32929
G	0	GLY	-	expression tag	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	PRO	-	expression tag	UNP P32929
G	59	ASN	GLU	engineered mutation	UNP P32929
G	119	LEU	ARG	engineered mutation	UNP P32929
G	339	VAL	GLU	engineered mutation	UNP P32929
H	-16	MET	-	expression tag	UNP P32929
H	-15	GLY	-	expression tag	UNP P32929
H	-14	GLY	-	expression tag	UNP P32929
H	-13	HIS	-	expression tag	UNP P32929
H	-12	HIS	-	expression tag	UNP P32929
H	-11	HIS	-	expression tag	UNP P32929
H	-10	HIS	-	expression tag	UNP P32929
H	-9	HIS	-	expression tag	UNP P32929
H	-8	HIS	-	expression tag	UNP P32929
H	-7	GLY	-	expression tag	UNP P32929
H	-6	LEU	-	expression tag	UNP P32929
H	-5	GLU	-	expression tag	UNP P32929
H	-4	VAL	-	expression tag	UNP P32929
H	-3	LEU	-	expression tag	UNP P32929
H	-2	PHE	-	expression tag	UNP P32929
H	-1	GLN	-	expression tag	UNP P32929
H	0	GLY	-	expression tag	UNP P32929
H	1	PRO	-	expression tag	UNP P32929
H	59	ASN	GLU	engineered mutation	UNP P32929
H	119	LEU	ARG	engineered mutation	UNP P32929
H	339	VAL	GLU	engineered mutation	UNP P32929

- Molecule 2 is a protein called Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	386	Total	C	N	O	S	0	0	0
			2984	1906	508	551	19			
2	E	385	Total	C	N	O	S	0	0	0
			2978	1903	507	549	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P32929
C	-15	GLY	-	expression tag	UNP P32929
C	-14	GLY	-	expression tag	UNP P32929
C	-13	HIS	-	expression tag	UNP P32929
C	-12	HIS	-	expression tag	UNP P32929

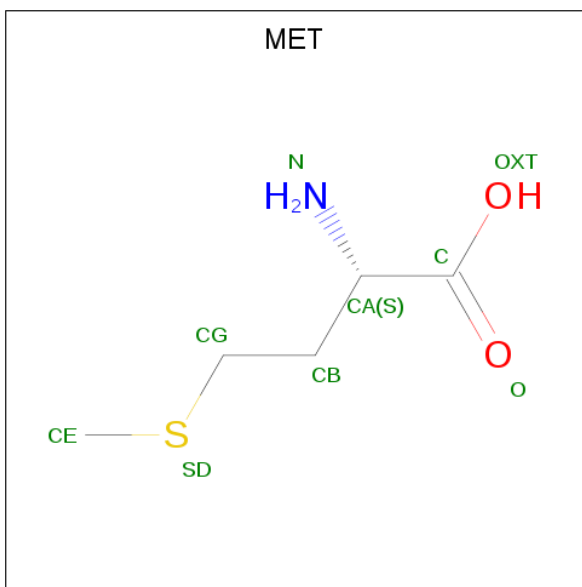
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	HIS	-	expression tag	UNP P32929
C	-10	HIS	-	expression tag	UNP P32929
C	-9	HIS	-	expression tag	UNP P32929
C	-8	HIS	-	expression tag	UNP P32929
C	-7	GLY	-	expression tag	UNP P32929
C	-6	LEU	-	expression tag	UNP P32929
C	-5	GLU	-	expression tag	UNP P32929
C	-4	VAL	-	expression tag	UNP P32929
C	-3	LEU	-	expression tag	UNP P32929
C	-2	PHE	-	expression tag	UNP P32929
C	-1	GLN	-	expression tag	UNP P32929
C	0	GLY	-	expression tag	UNP P32929
C	1	PRO	-	expression tag	UNP P32929
C	59	ASN	GLU	engineered mutation	UNP P32929
C	119	LEU	ARG	engineered mutation	UNP P32929
C	339	VAL	GLU	engineered mutation	UNP P32929
E	-16	MET	-	initiating methionine	UNP P32929
E	-15	GLY	-	expression tag	UNP P32929
E	-14	GLY	-	expression tag	UNP P32929
E	-13	HIS	-	expression tag	UNP P32929
E	-12	HIS	-	expression tag	UNP P32929
E	-11	HIS	-	expression tag	UNP P32929
E	-10	HIS	-	expression tag	UNP P32929
E	-9	HIS	-	expression tag	UNP P32929
E	-8	HIS	-	expression tag	UNP P32929
E	-7	GLY	-	expression tag	UNP P32929
E	-6	LEU	-	expression tag	UNP P32929
E	-5	GLU	-	expression tag	UNP P32929
E	-4	VAL	-	expression tag	UNP P32929
E	-3	LEU	-	expression tag	UNP P32929
E	-2	PHE	-	expression tag	UNP P32929
E	-1	GLN	-	expression tag	UNP P32929
E	0	GLY	-	expression tag	UNP P32929
E	1	PRO	-	expression tag	UNP P32929
E	59	ASN	GLU	engineered mutation	UNP P32929
E	119	LEU	ARG	engineered mutation	UNP P32929
E	339	VAL	GLU	engineered mutation	UNP P32929

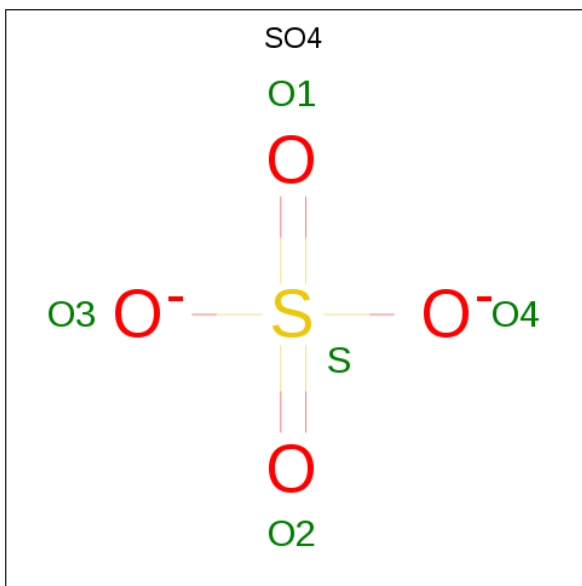
- Molecule 3 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).





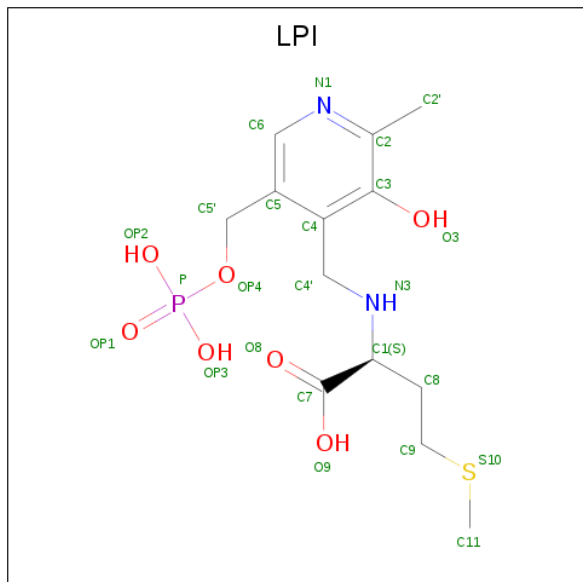
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

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



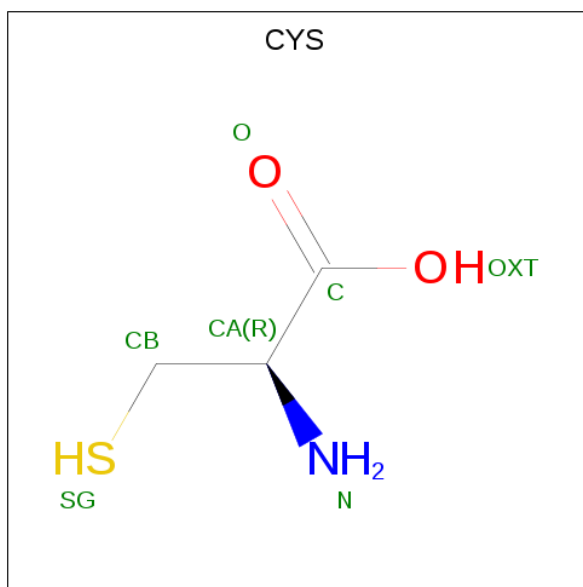
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)-L-methionine (three-letter code: LPI) (formula:  $C_{13}H_{21}N_2O_7PS$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
5	E	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		

- Molecule 6 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
6	G	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
6	H	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

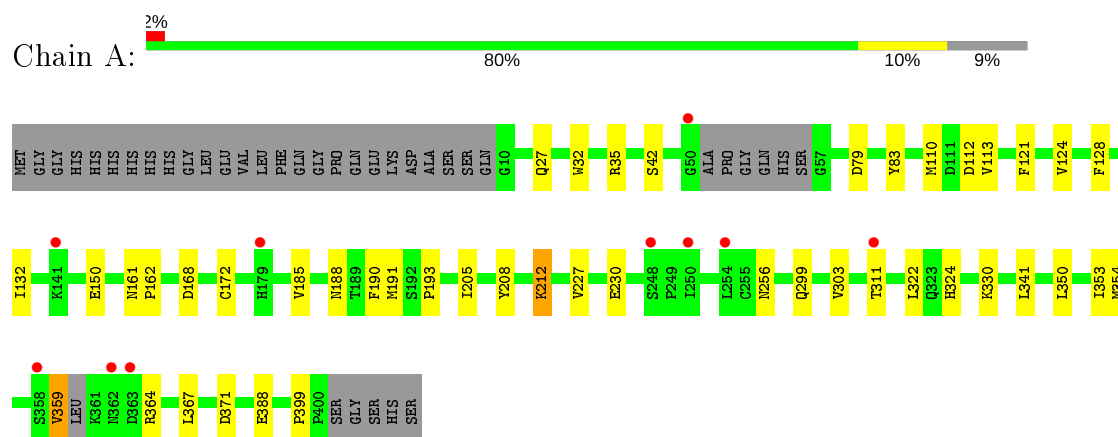
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	177	Total	O	0	0
			177	177		
7	B	139	Total	O	0	0
			139	139		
7	C	176	Total	O	0	0
			176	176		
7	D	157	Total	O	0	0
			157	157		
7	E	103	Total	O	0	0
			103	103		
7	F	63	Total	O	0	0
			63	63		
7	G	94	Total	O	0	0
			94	94		
7	H	103	Total	O	0	0
			103	103		

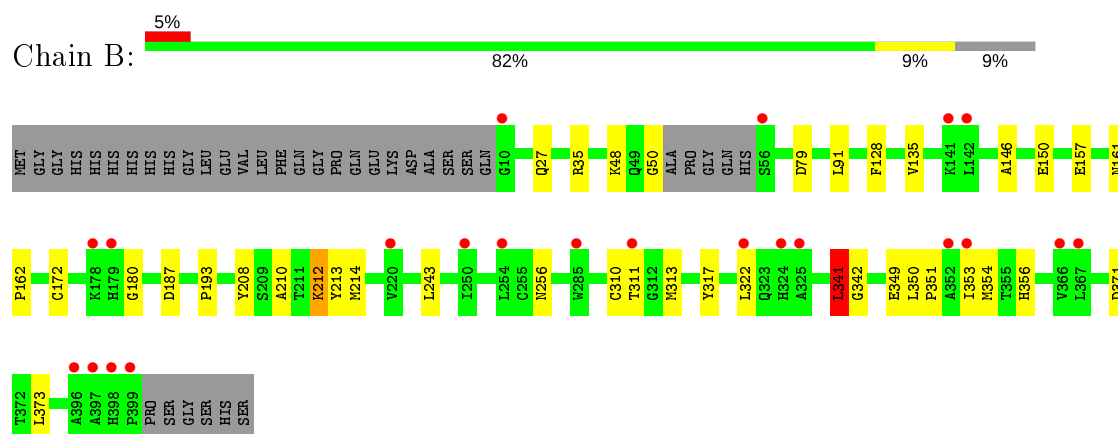
### 3 Residue-property plots [i](#)

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.

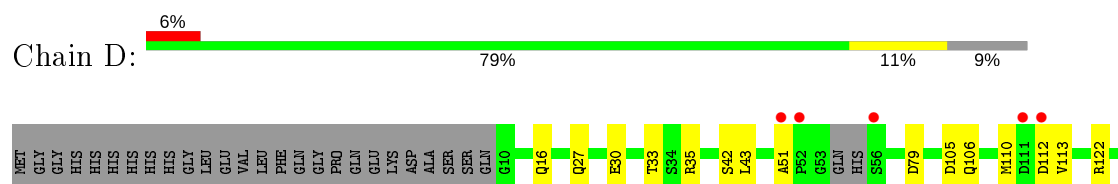
#### • Molecule 1: Cystathionine gamma-lyase

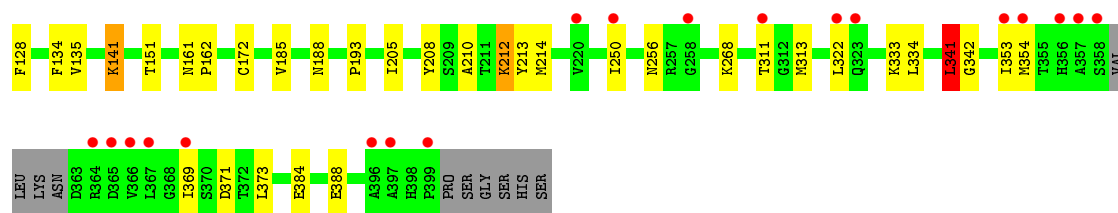


#### • Molecule 1: Cystathionine gamma-lyase

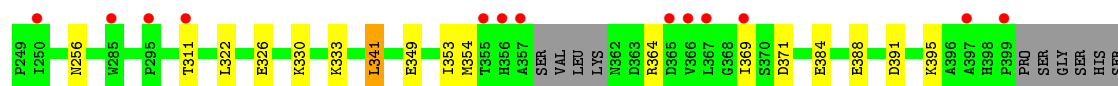
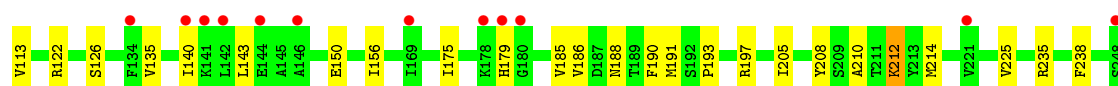
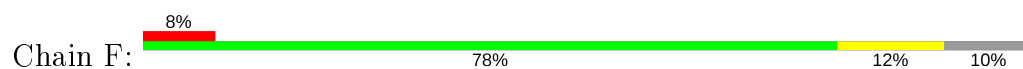


#### • Molecule 1: Cystathionine gamma-lyase

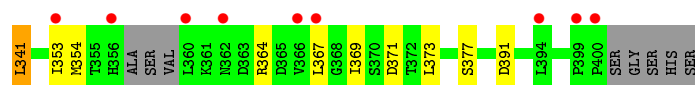
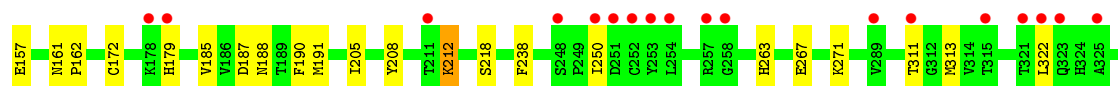
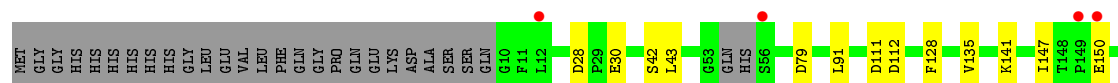
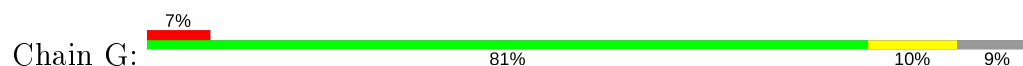




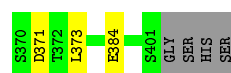
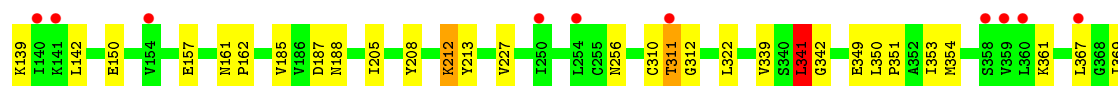
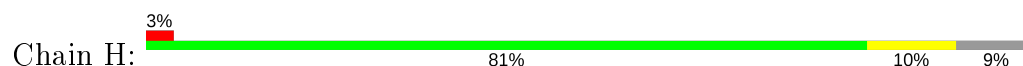
• Molecule 1: Cystathionine gamma-lyase



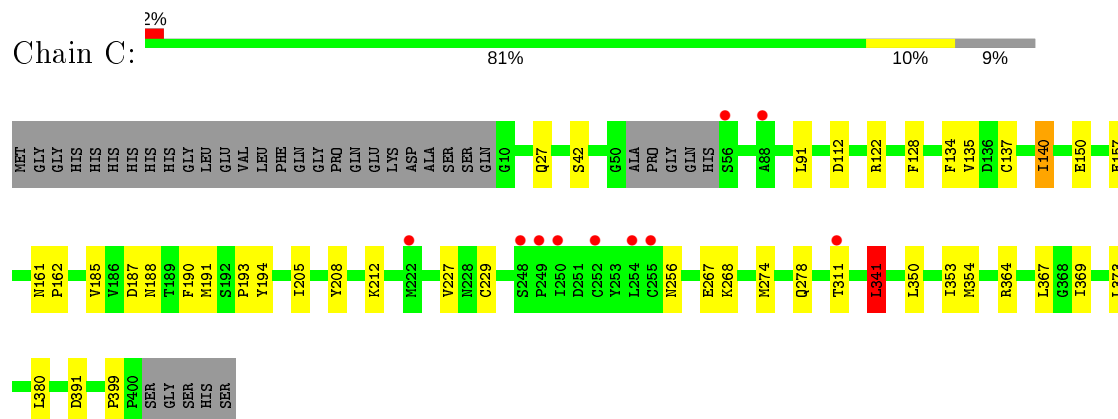
• Molecule 1: Cystathionine gamma-lyase



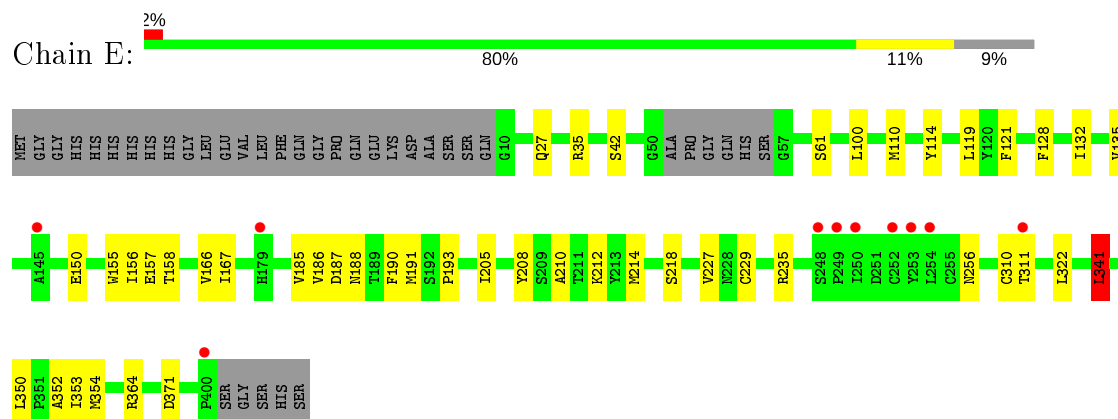
• Molecule 1: Cystathionine gamma-lyase



- Molecule 2: Cystathionine gamma-lyase



- Molecule 2: Cystathionine gamma-lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.89Å 163.68Å 181.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.20 49.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.04-2.20) 95.7 (49.04-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.171 , 0.202 0.175 , 0.204	Depositor DCC
$R_{free}$ test set	8040 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	24978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.31	0/3026	0.50	1/4105 (0.0%)
1	B	0.28	0/3033	0.47	1/4115 (0.0%)
1	D	0.28	0/3017	0.47	1/4093 (0.0%)
1	F	0.26	0/3001	0.46	0/4071
1	G	0.27	0/3038	0.46	0/4122
1	H	0.28	0/3043	0.46	1/4130 (0.0%)
2	C	0.29	0/3051	0.50	1/4141 (0.0%)
2	E	0.27	0/3045	0.47	1/4133 (0.0%)
All	All	0.28	0/24254	0.47	6/32910 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	341	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	359	VAL	N-CA-C	-5.86	95.18	111.00
2	E	341	LEU	CA-CB-CG	5.79	128.61	115.30
1	B	341	LEU	CA-CB-CG	5.17	127.18	115.30
1	H	341	LEU	CA-CB-CG	5.12	127.07	115.30
1	D	341	LEU	CA-CB-CG	5.01	126.82	115.30

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	2985	0	2974	32	0
1	B	2992	0	2983	27	0
1	D	2976	0	2959	33	0
1	F	2961	0	2945	37	0
1	G	2996	0	2984	33	0
1	H	3001	0	2993	34	0
2	C	2984	0	2986	30	0
2	E	2978	0	2982	33	0
3	A	9	0	8	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	C	24	0	0	0	0
5	E	24	0	0	3	0
6	F	7	0	4	1	0
6	G	7	0	4	0	0
6	H	7	0	4	3	0
7	A	177	0	0	4	0
7	B	139	0	0	1	0
7	C	176	0	0	4	0
7	D	157	0	0	6	0
7	E	103	0	0	5	0
7	F	63	0	0	4	0
7	G	94	0	0	7	0
7	H	103	0	0	5	0
All	All	24978	0	23826	248	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 5.

All (248) 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:G:157:GLU:HG2	1:G:187:ASP:HB3	1.35	1.03
1:H:157:GLU:HG2	1:H:187:ASP:HB3	1.45	0.98
1:G:391:ASP:OD1	7:G:601:HOH:O	1.88	0.90
1:H:212:LLP:H4'1	6:H:501:CYS:N	1.90	0.86
1:F:47:PHE:O	7:F:601:HOH:O	1.95	0.83
2:E:218:SER:OG	7:E:601:HOH:O	1.97	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLU:OE1	7:A:601:HOH:O	1.97	0.81
1:B:311:THR:HG23	1:B:313:MET:H	1.47	0.80
1:D:311:THR:HG23	1:D:313:MET:H	1.46	0.80
2:E:229:CYS:SG	7:E:699:HOH:O	2.21	0.79
1:F:353:ILE:HG13	1:F:354:MET:HG3	1.64	0.78
1:D:79:ASP:OD1	7:D:601:HOH:O	2.01	0.77
1:G:30:GLU:OE1	7:G:602:HOH:O	2.03	0.77
1:G:218:SER:OG	7:G:603:HOH:O	2.03	0.76
2:C:191:MET:HA	2:C:311:THR:HG21	1.66	0.76
1:B:180:GLY:O	7:B:601:HOH:O	2.03	0.75
1:F:191:MET:HA	1:F:311:THR:HG21	1.67	0.75
1:F:388:GLU:OE2	7:F:602:HOH:O	2.05	0.75
1:D:353:ILE:HG13	1:D:354:MET:HG3	1.68	0.74
1:B:157:GLU:HG2	1:B:187:ASP:HB3	1.71	0.72
1:D:105:ASP:OD2	7:D:602:HOH:O	2.07	0.72
2:C:229:CYS:SG	7:C:775:HOH:O	2.47	0.72
1:D:268:LYS:NZ	7:D:607:HOH:O	2.24	0.70
2:C:353:ILE:HG23	2:C:354:MET:HG3	1.72	0.70
2:E:190:PHE:O	2:E:311:THR:HG21	1.93	0.68
1:G:191:MET:HA	1:G:311:THR:HG21	1.74	0.68
1:F:391:ASP:OD2	1:F:395:LYS:NZ	2.28	0.67
1:B:212:LLP:HB2	1:B:341:LEU:HD22	1.77	0.66
2:C:364:ARG:HG2	2:C:369:ILE:HB	1.77	0.66
2:E:353:ILE:HG13	2:E:354:MET:HG3	1.78	0.66
1:A:191:MET:HA	1:A:311:THR:HG21	1.76	0.66
1:F:212:LLP:H4'1	6:F:501:CYS:N	2.11	0.66
2:C:212:LYS:HB3	2:C:341:LEU:HD22	1.79	0.65
1:D:16:GLN:OE1	7:D:603:HOH:O	2.13	0.65
1:G:79:ASP:OD1	1:G:208:TYR:OH	2.11	0.65
2:E:191:MET:HA	2:E:311:THR:HG21	1.79	0.64
1:B:322:LEU:HB2	1:B:371:ASP:HB3	1.80	0.64
2:E:352:ALA:O	2:E:364:ARG:NH1	2.31	0.64
1:F:140:ILE:HD12	1:F:143:LEU:HB3	1.78	0.64
1:F:190:PHE:O	1:F:311:THR:HG21	1.98	0.64
1:B:212:LLP:HD3	1:B:341:LEU:HD13	1.81	0.62
1:A:212:LLP:H4'1	3:A:501:MET:N	2.14	0.62
1:A:32:TRP:O	1:A:35:ARG:NH1	2.32	0.62
1:H:361:LYS:N	7:H:605:HOH:O	2.34	0.61
2:C:190:PHE:O	2:C:311:THR:HG21	2.00	0.61
1:G:212:LLP:HB2	1:G:341:LEU:HD22	1.84	0.60
1:H:212:LLP:C4'	6:H:501:CYS:N	2.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:311:THR:OG1	1:H:312:GLY:N	2.32	0.60
2:E:157:GLU:HG2	2:E:187:ASP:HB3	1.82	0.60
1:F:110:MET:HB3	1:F:113:VAL:HG13	1.83	0.60
2:E:114:TYR:OH	5:E:501:LPI:S10	2.46	0.60
2:C:157:GLU:HG2	2:C:187:ASP:HB3	1.84	0.59
1:D:388:GLU:OE1	7:D:604:HOH:O	2.17	0.59
2:E:100:LEU:O	2:E:235:ARG:NH2	2.36	0.59
1:F:384:GLU:OE1	1:F:384:GLU:N	2.31	0.59
1:H:212:LLP:HD3	1:H:341:LEU:HD13	1.84	0.59
1:G:369:ILE:HA	1:G:373:LEU:HD22	1.84	0.58
1:A:190:PHE:O	1:A:311:THR:HG21	2.03	0.58
1:H:212:LLP:HB2	1:H:341:LEU:HD22	1.85	0.57
2:E:212:LYS:HE3	5:E:501:LPI:C4'	2.35	0.57
1:A:168:ASP:OD2	7:A:602:HOH:O	2.18	0.57
1:H:213:TYR:HH	1:H:311:THR:HG1	1.51	0.57
1:G:190:PHE:O	1:G:311:THR:HG21	2.05	0.57
1:H:185:VAL:HG22	1:H:205:ILE:HB	1.86	0.57
1:H:112:ASP:HB2	1:H:367:LEU:HD22	1.87	0.56
1:H:139:LYS:HB2	1:H:142:LEU:HD13	1.88	0.56
1:F:388:GLU:HG3	7:F:602:HOH:O	2.05	0.56
1:H:353:ILE:HG13	1:H:354:MET:HG3	1.88	0.56
1:D:212:LLP:HD3	1:D:341:LEU:HD13	1.88	0.55
1:A:359:VAL:HG12	1:A:364:ARG:HG3	1.88	0.55
2:E:119:LEU:HD21	1:F:238:PHE:CZ	2.42	0.55
1:F:156:ILE:HD11	1:F:186:VAL:HG22	1.90	0.54
1:A:27:GLN:HE22	1:A:256:ASN:HD21	1.55	0.54
1:A:353:ILE:HG13	1:A:354:MET:HG3	1.88	0.54
1:A:83:TYR:OH	1:A:230:GLU:OE2	2.19	0.54
2:C:150:GLU:OE2	2:C:150:GLU:N	2.41	0.53
1:B:135:VAL:HG11	1:B:146:ALA:HB2	1.90	0.53
1:D:110:MET:HB2	1:D:113:VAL:HG13	1.90	0.53
2:E:35:ARG:NE	7:E:611:HOH:O	2.42	0.53
1:F:191:MET:HA	1:F:311:THR:CG2	2.38	0.53
1:G:353:ILE:HG13	1:G:354:MET:HG3	1.91	0.53
1:G:150:GLU:OE1	1:G:150:GLU:N	2.43	0.52
2:C:212:LYS:HD2	2:C:341:LEU:HD13	1.91	0.52
1:A:205:ILE:HG12	1:A:227:VAL:HG12	1.91	0.52
2:E:150:GLU:OE1	2:E:150:GLU:N	2.42	0.52
2:C:122:ARG:HG3	2:C:134:PHE:HE2	1.74	0.52
1:G:128:PHE:HB3	1:H:128:PHE:HB3	1.91	0.52
1:H:122:ARG:NH1	7:H:610:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:LLP:HD3	1:F:341:LEU:HD13	1.91	0.52
1:A:150:GLU:N	1:A:150:GLU:OE2	2.43	0.51
1:B:27:GLN:HE22	1:B:256:ASN:HD21	1.57	0.51
1:F:212:LLP:HB2	1:F:341:LEU:HD22	1.92	0.51
1:A:110:MET:HB2	1:A:113:VAL:HG13	1.91	0.51
1:B:79:ASP:OD1	1:B:208:TYR:OH	2.23	0.51
1:D:27:GLN:HE22	1:D:256:ASN:HD21	1.58	0.51
2:E:27:GLN:HE22	2:E:256:ASN:HD21	1.58	0.51
1:F:185:VAL:HG22	1:F:205:ILE:HB	1.92	0.51
1:F:322:LEU:HB2	1:F:371:ASP:HB3	1.91	0.51
2:C:42:SER:HB3	7:C:626:HOH:O	2.11	0.51
1:A:112:ASP:HB2	1:A:367:LEU:HD22	1.91	0.51
1:G:212:LLP:HD3	1:G:341:LEU:HD13	1.92	0.51
2:E:212:LYS:CE	5:E:501:LPI:C4'	2.89	0.50
1:G:322:LEU:HB2	1:G:371:ASP:HB3	1.93	0.50
1:B:317:TYR:CZ	1:B:373:LEU:HD12	2.47	0.50
2:E:110:MET:SD	2:E:167:ILE:HD11	2.51	0.50
1:G:263:HIS:ND1	7:G:607:HOH:O	2.34	0.50
1:F:364:ARG:HB2	1:F:369:ILE:HB	1.93	0.50
1:F:188:ASN:HB3	1:F:208:TYR:CE2	2.46	0.50
1:B:48:LYS:NZ	1:D:30:GLU:OE2	2.33	0.49
1:D:212:LLP:HB2	1:D:341:LEU:HD22	1.93	0.49
1:A:42:SER:HB3	7:A:640:HOH:O	2.13	0.49
2:E:42:SER:HB3	7:E:616:HOH:O	2.12	0.49
2:C:391:ASP:OD1	7:C:601:HOH:O	2.20	0.49
2:E:212:LYS:HB3	2:E:341:LEU:HD22	1.95	0.49
1:H:150:GLU:OE1	1:H:150:GLU:N	2.43	0.49
1:H:81:ALA:O	7:H:602:HOH:O	2.20	0.49
1:B:150:GLU:OE1	1:B:150:GLU:N	2.45	0.49
2:E:185:VAL:HG22	2:E:205:ILE:HB	1.95	0.49
1:H:310:CYS:SG	1:H:311:THR:N	2.85	0.48
1:F:27:GLN:HE22	1:F:256:ASN:HD21	1.59	0.48
1:A:79:ASP:OD1	1:A:208:TYR:OH	2.21	0.48
1:H:384:GLU:HB3	7:H:695:HOH:O	2.14	0.48
2:C:274:MET:O	2:C:278:GLN:HG3	2.14	0.47
1:A:188:ASN:HB3	1:A:208:TYR:CE2	2.49	0.47
1:H:322:LEU:HB2	1:H:371:ASP:HB3	1.96	0.47
2:E:188:ASN:HB3	2:E:208:TYR:CE2	2.50	0.47
1:H:121:PHE:HB3	1:H:132:ILE:HG21	1.96	0.47
1:H:69:ASN:OD1	7:H:603:HOH:O	2.20	0.47
1:A:128:PHE:HB3	1:B:128:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:MET:HE1	1:G:377:SER:OG	2.13	0.47
1:G:188:ASN:HB3	1:G:208:TYR:CE2	2.50	0.47
1:H:188:ASN:HB3	1:H:208:TYR:CE2	2.50	0.47
1:H:21:GLN:NE2	1:H:77:ALA:HB1	2.30	0.47
1:F:140:ILE:HD11	1:F:175:ILE:HG21	1.97	0.47
1:G:30:GLU:OE1	1:G:30:GLU:N	2.47	0.47
2:E:158:THR:HG23	2:E:166:VAL:HA	1.95	0.46
2:C:185:VAL:HG22	2:C:205:ILE:HB	1.98	0.46
1:A:212:LLP:C4'	3:A:501:MET:N	2.78	0.46
2:C:122:ARG:HG3	2:C:134:PHE:CE2	2.50	0.46
1:D:210:ALA:HA	1:D:214:MET:HB2	1.97	0.46
1:G:112:ASP:HB2	1:G:367:LEU:HD22	1.96	0.46
1:A:324:HIS:CG	1:A:399:PRO:HB3	2.50	0.46
2:C:191:MET:HA	2:C:311:THR:CG2	2.41	0.46
1:A:191:MET:HA	1:A:311:THR:CG2	2.43	0.46
1:D:161:ASN:HA	1:D:162:PRO:HA	1.78	0.46
1:D:141:LYS:HD2	1:D:141:LYS:HA	1.71	0.46
1:H:369:ILE:HA	1:H:373:LEU:HD22	1.96	0.46
1:A:350:LEU:HD23	1:A:353:ILE:H	1.80	0.45
2:C:369:ILE:HA	2:C:373:LEU:HD22	1.98	0.45
1:F:333:LYS:HE3	1:F:333:LYS:HB2	1.81	0.45
1:G:111:ASP:OD1	1:G:112:ASP:N	2.49	0.45
1:G:364:ARG:HG2	1:G:369:ILE:O	2.16	0.45
1:D:112:ASP:OD1	1:D:112:ASP:N	2.48	0.45
1:A:124:VAL:HG11	1:B:243:LEU:HD21	1.97	0.45
1:A:193:PRO:HD3	1:A:208:TYR:CE2	2.52	0.45
2:C:194:TYR:OH	2:C:267:GLU:OE1	2.25	0.45
1:G:42:SER:HB3	7:G:631:HOH:O	2.16	0.45
1:A:185:VAL:HG22	1:A:205:ILE:HB	1.98	0.45
1:G:141:LYS:HD2	1:G:141:LYS:H	1.82	0.45
1:D:30:GLU:OE1	1:D:30:GLU:N	2.48	0.45
2:C:350:LEU:HD23	2:C:353:ILE:H	1.82	0.44
1:A:322:LEU:HB2	1:A:371:ASP:HB3	1.99	0.44
1:B:161:ASN:O	1:B:356:HIS:NE2	2.51	0.44
2:C:128:PHE:HB3	1:D:128:PHE:HB3	1.98	0.44
2:C:399:PRO:HB2	1:F:384:GLU:HB2	1.99	0.44
1:D:213:TYR:CZ	1:D:311:THR:OG1	2.69	0.44
1:D:384:GLU:H	1:D:384:GLU:CD	2.19	0.44
2:E:310:CYS:SG	2:E:311:THR:N	2.90	0.44
1:H:213:TYR:CE1	1:H:342:GLY:HA2	2.53	0.44
2:C:256:ASN:HB3	7:C:739:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:HIS:CD2	1:A:399:PRO:HB3	2.53	0.44
1:B:310:CYS:SG	1:B:311:THR:N	2.91	0.44
1:D:188:ASN:HB3	1:D:208:TYR:CE2	2.52	0.44
1:G:267:GLU:O	1:G:271:LYS:HG3	2.18	0.44
1:D:122:ARG:HG3	1:D:134:PHE:CE1	2.53	0.44
1:G:161:ASN:HA	1:G:162:PRO:HA	1.77	0.44
2:E:61:SER:OG	7:E:603:HOH:O	2.21	0.43
1:H:349:GLU:OE2	1:H:351:PRO:HA	2.18	0.43
1:D:334:LEU:HD23	1:D:334:LEU:HA	1.85	0.43
2:E:128:PHE:HA	1:F:103:ALA:HB2	1.99	0.43
1:F:100:LEU:O	1:F:235:ARG:NH2	2.50	0.43
1:G:191:MET:HA	1:G:311:THR:CG2	2.45	0.43
2:C:112:ASP:HB2	2:C:367:LEU:HD22	1.99	0.43
2:E:191:MET:HA	2:E:311:THR:CG2	2.45	0.43
1:A:256:ASN:HB3	7:A:732:HOH:O	2.19	0.43
1:B:349:GLU:OE2	1:B:351:PRO:HA	2.18	0.43
1:D:193:PRO:HD3	1:D:208:TYR:CE2	2.53	0.43
1:B:35:ARG:HH11	1:D:51:ALA:HB3	1.83	0.43
1:H:350:LEU:HD23	1:H:353:ILE:HG23	2.00	0.43
2:E:193:PRO:HD3	2:E:208:TYR:CE2	2.53	0.43
1:F:140:ILE:CD1	1:F:175:ILE:HD13	2.49	0.43
2:C:161:ASN:HA	2:C:162:PRO:HA	1.85	0.43
1:G:147:ILE:HG21	1:G:179:HIS:CD2	2.54	0.43
1:H:213:TYR:OH	1:H:311:THR:OG1	2.26	0.43
1:A:161:ASN:HA	1:A:162:PRO:HA	1.81	0.43
1:B:161:ASN:HA	1:B:162:PRO:HA	1.83	0.43
1:B:50:GLY:N	1:D:35:ARG:HH22	2.17	0.43
2:C:137:CYS:O	2:C:140:ILE:HD13	2.19	0.43
1:H:139:LYS:CB	1:H:142:LEU:HD13	2.49	0.43
2:C:188:ASN:HB3	2:C:208:TYR:CE2	2.54	0.42
2:E:322:LEU:HB2	2:E:371:ASP:HB3	2.00	0.42
1:F:150:GLU:N	1:F:150:GLU:OE1	2.52	0.42
1:H:136:ASP:HB3	1:H:142:LEU:HD23	2.01	0.42
2:E:350:LEU:HD23	2:E:353:ILE:HG23	2.01	0.42
1:G:191:MET:HG2	7:G:617:HOH:O	2.19	0.42
1:G:185:VAL:HG22	1:G:205:ILE:HB	2.02	0.42
1:H:161:ASN:HA	1:H:162:PRO:HA	1.79	0.42
2:E:121:PHE:O	2:E:132:ILE:HG13	2.18	0.42
1:G:43:LEU:HD21	1:G:250:ILE:HG12	2.01	0.42
1:B:353:ILE:HG13	1:B:354:MET:HG3	2.01	0.42
1:A:330:LYS:HA	1:A:330:LYS:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:LEU:HA	2:C:91:LEU:HD23	1.92	0.42
1:F:384:GLU:CD	1:F:384:GLU:H	2.15	0.42
1:B:213:TYR:CE1	1:B:342:GLY:HA2	2.54	0.41
2:E:156:ILE:HD11	2:E:186:VAL:HG22	2.02	0.41
1:B:213:TYR:CZ	1:B:311:THR:OG1	2.69	0.41
2:C:193:PRO:HD3	2:C:208:TYR:CE2	2.55	0.41
1:D:185:VAL:HG22	1:D:205:ILE:HB	2.02	0.41
1:F:110:MET:HG3	1:F:112:ASP:H	1.85	0.41
1:F:205:ILE:HG23	1:F:225:VAL:HG13	2.02	0.41
2:C:27:GLN:HE22	2:C:256:ASN:HD21	1.68	0.41
1:F:193:PRO:HD3	1:F:208:TYR:CE2	2.55	0.41
2:E:193:PRO:HD3	2:E:208:TYR:CZ	2.55	0.41
1:A:121:PHE:HB3	1:A:132:ILE:HG21	2.03	0.41
1:A:299:GLN:O	1:A:303:VAL:HG23	2.19	0.41
1:D:106:GLN:HB3	1:D:151:THR:HA	2.02	0.41
1:D:369:ILE:HA	1:D:373:LEU:HD22	2.02	0.41
1:H:27:GLN:HE22	1:H:256:ASN:HD21	1.68	0.41
1:B:350:LEU:HD22	1:B:353:ILE:HG23	2.03	0.41
1:D:42:SER:HB3	7:D:665:HOH:O	2.20	0.41
1:F:122:ARG:O	1:F:126:SER:OG	2.23	0.41
1:G:28:ASP:HB3	7:G:602:HOH:O	2.21	0.41
2:C:268:LYS:HB3	2:C:380:LEU:HD22	2.02	0.41
1:D:322:LEU:HB2	1:D:371:ASP:HB3	2.02	0.41
1:G:238:PHE:CZ	1:H:119:LEU:HD21	2.55	0.41
1:H:339:VAL:HB	6:H:501:CYS:HB2	2.02	0.41
2:E:155:TRP:CZ3	2:E:185:VAL:HG11	2.56	0.41
1:B:91:LEU:HA	1:B:91:LEU:HD23	1.95	0.40
1:D:43:LEU:HD21	1:D:250:ILE:HG12	2.04	0.40
1:F:210:ALA:HA	1:F:214:MET:HB2	2.02	0.40
1:B:210:ALA:HA	1:B:214:MET:HB2	2.02	0.40
1:D:213:TYR:CE1	1:D:342:GLY:HA2	2.56	0.40
1:F:197:ARG:NH2	7:F:605:HOH:O	2.35	0.40
1:F:32:TRP:CZ2	1:F:39:PRO:HB3	2.57	0.40
1:F:326:GLU:O	1:F:330:LYS:HD3	2.21	0.40
1:G:91:LEU:HD23	1:G:91:LEU:HA	1.88	0.40
1:B:193:PRO:HD3	1:B:208:TYR:CE2	2.57	0.40
2:E:210:ALA:HA	2:E:214:MET:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	377/422 (89%)	365 (97%)	12 (3%)	0	100	100
1	B	380/422 (90%)	371 (98%)	9 (2%)	0	100	100
1	D	377/422 (89%)	367 (97%)	10 (3%)	0	100	100
1	F	374/422 (89%)	363 (97%)	11 (3%)	0	100	100
1	G	379/422 (90%)	371 (98%)	8 (2%)	0	100	100
1	H	381/422 (90%)	373 (98%)	8 (2%)	0	100	100
2	C	382/422 (90%)	372 (97%)	10 (3%)	0	100	100
2	E	381/422 (90%)	372 (98%)	9 (2%)	0	100	100
All	All	3031/3376 (90%)	2954 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/356 (92%)	324 (99%)	2 (1%)	86	93
1	B	327/356 (92%)	325 (99%)	2 (1%)	86	93
1	D	324/356 (91%)	318 (98%)	6 (2%)	57	71
1	F	322/356 (90%)	317 (98%)	5 (2%)	62	76
1	G	327/356 (92%)	324 (99%)	3 (1%)	78	88
1	H	329/356 (92%)	326 (99%)	3 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	329/357 (92%)	325 (99%)	4 (1%)	71	83
2	E	328/357 (92%)	325 (99%)	3 (1%)	78	88
All	All	2612/2850 (92%)	2584 (99%)	28 (1%)	73	85

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	CYS
1	A	341	LEU
1	B	172	CYS
1	B	341	LEU
2	C	135	VAL
2	C	140	ILE
2	C	227	VAL
2	C	341	LEU
1	D	33	THR
1	D	135	VAL
1	D	141	LYS
1	D	172	CYS
1	D	333	LYS
1	D	341	LEU
2	E	135	VAL
2	E	227	VAL
2	E	341	LEU
1	F	59	ASN
1	F	135	VAL
1	F	179	HIS
1	F	341	LEU
1	F	349	GLU
1	G	135	VAL
1	G	172	CYS
1	G	341	LEU
1	H	227	VAL
1	H	311	THR
1	H	341	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN

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Mol	Chain	Res	Type
1	B	123	GLN
1	B	256	ASN
2	C	256	ASN
1	D	256	ASN
1	D	356	HIS
1	D	398	HIS
2	E	106	GLN
2	E	256	ASN
1	F	256	ASN
1	G	106	GLN
1	G	179	HIS
1	G	398	HIS
1	H	256	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	G	212	1	23,24,25	2.63	6 (26%)	25,32,34	1.20	3 (12%)
1	LLP	A	212	1	23,24,25	2.60	5 (21%)	25,32,34	1.33	2 (8%)
1	LLP	F	212	1	23,24,25	2.66	5 (21%)	25,32,34	1.18	3 (12%)
1	LLP	H	212	1	23,24,25	2.69	6 (26%)	25,32,34	1.20	3 (12%)
1	LLP	B	212	1,4	23,24,25	2.73	6 (26%)	25,32,34	1.25	2 (8%)
1	LLP	D	212	1	23,24,25	2.58	6 (26%)	25,32,34	1.25	3 (12%)

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
1	LLP	G	212	1	-	6/16/17/19	0/1/1/1
1	LLP	A	212	1	-	7/16/17/19	0/1/1/1
1	LLP	F	212	1	-	8/16/17/19	0/1/1/1
1	LLP	H	212	1	-	7/16/17/19	0/1/1/1
1	LLP	B	212	1,4	-	10/16/17/19	0/1/1/1
1	LLP	D	212	1	-	4/16/17/19	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	LLP	C4-C4'	8.92	1.63	1.46
1	A	212	LLP	C4-C4'	8.50	1.62	1.46
1	F	212	LLP	C4-C4'	8.47	1.62	1.46
1	H	212	LLP	C4-C4'	8.44	1.62	1.46
1	G	212	LLP	C4-C4'	8.21	1.62	1.46
1	D	212	LLP	C4-C4'	8.19	1.62	1.46
1	A	212	LLP	C4'-NZ	5.36	1.45	1.27
1	H	212	LLP	C4'-NZ	5.35	1.45	1.27
1	B	212	LLP	C4'-NZ	5.31	1.45	1.27
1	F	212	LLP	C4'-NZ	5.16	1.44	1.27
1	G	212	LLP	C4'-NZ	5.15	1.44	1.27
1	D	212	LLP	C4'-NZ	5.08	1.44	1.27
1	F	212	LLP	C4-C5	-3.82	1.37	1.42
1	G	212	LLP	C4-C5	-3.71	1.37	1.42
1	H	212	LLP	C4-C5	-3.63	1.37	1.42
1	G	212	LLP	C2'-C2	3.61	1.56	1.50
1	H	212	LLP	C2'-C2	3.50	1.56	1.50
1	D	212	LLP	C4-C5	-3.48	1.37	1.42
1	F	212	LLP	C2'-C2	3.48	1.56	1.50
1	B	212	LLP	C2'-C2	3.48	1.56	1.50
1	D	212	LLP	C2'-C2	3.47	1.56	1.50
1	B	212	LLP	C4-C5	-3.47	1.37	1.42
1	A	212	LLP	C2'-C2	3.36	1.56	1.50
1	B	212	LLP	C6-N1	3.11	1.41	1.34
1	A	212	LLP	C4-C5	-3.11	1.38	1.42
1	H	212	LLP	C6-N1	3.08	1.40	1.34
1	G	212	LLP	C6-N1	3.03	1.40	1.34
1	F	212	LLP	C6-N1	2.88	1.40	1.34
1	D	212	LLP	C6-N1	2.85	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	LLP	C6-N1	2.79	1.40	1.34
1	D	212	LLP	C5'-C5	2.26	1.57	1.50
1	G	212	LLP	C5'-C5	2.16	1.56	1.50
1	H	212	LLP	C5'-C5	2.08	1.56	1.50
1	B	212	LLP	C3-C2	2.08	1.43	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LLP	C4-C4'-NZ	-3.55	108.01	124.31
1	D	212	LLP	C4-C4'-NZ	-3.51	108.20	124.31
1	B	212	LLP	C4-C4'-NZ	-3.22	109.50	124.31
1	H	212	LLP	C4-C4'-NZ	-3.15	109.83	124.31
1	F	212	LLP	C4-C4'-NZ	-3.11	110.02	124.31
1	G	212	LLP	C4-C4'-NZ	-3.10	110.09	124.31
1	F	212	LLP	C5-C6-N1	-2.53	119.60	123.82
1	G	212	LLP	CE-NZ-C4'	-2.43	111.45	118.90
1	F	212	LLP	CE-NZ-C4'	-2.41	111.51	118.90
1	A	212	LLP	C5-C6-N1	-2.32	119.96	123.82
1	D	212	LLP	CE-NZ-C4'	-2.25	112.00	118.90
1	H	212	LLP	CE-NZ-C4'	-2.23	112.04	118.90
1	G	212	LLP	C5-C6-N1	-2.21	120.14	123.82
1	H	212	LLP	C5-C6-N1	-2.18	120.19	123.82
1	D	212	LLP	C5-C6-N1	-2.12	120.30	123.82
1	B	212	LLP	C5-C6-N1	-2.05	120.40	123.82

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	212	LLP	C4-C4'-NZ-CE
1	G	212	LLP	N-CA-CB-CG
1	G	212	LLP	O-C-CA-CB
1	A	212	LLP	O-C-CA-CB
1	F	212	LLP	C4-C4'-NZ-CE
1	F	212	LLP	C4-C5-C5'-OP4
1	F	212	LLP	O-C-CA-CB
1	H	212	LLP	O-C-CA-CB
1	B	212	LLP	C4-C4'-NZ-CE
1	B	212	LLP	C5'-OP4-P-OP2
1	B	212	LLP	C5'-OP4-P-OP3
1	B	212	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	D	212	LLP	O-C-CA-CB
1	H	212	LLP	C4-C4'-NZ-CE
1	D	212	LLP	C4-C4'-NZ-CE
1	A	212	LLP	CG-CD-CE-NZ
1	A	212	LLP	C4-C4'-NZ-CE
1	B	212	LLP	C5'-OP4-P-OP1
1	B	212	LLP	CG-CD-CE-NZ
1	B	212	LLP	C3-C4-C4'-NZ
1	F	212	LLP	C6-C5-C5'-OP4
1	F	212	LLP	CG-CD-CE-NZ
1	H	212	LLP	C4-C5-C5'-OP4
1	A	212	LLP	CD-CE-NZ-C4'
1	H	212	LLP	CD-CE-NZ-C4'
1	B	212	LLP	CD-CE-NZ-C4'
1	F	212	LLP	N-CA-CB-CG
1	B	212	LLP	N-CA-CB-CG
1	D	212	LLP	N-CA-CB-CG
1	D	212	LLP	CD-CE-NZ-C4'
1	F	212	LLP	C3-C4-C4'-NZ
1	G	212	LLP	CD-CE-NZ-C4'
1	A	212	LLP	CA-CB-CG-CD
1	F	212	LLP	CD-CE-NZ-C4'
1	G	212	LLP	C3-C4-C4'-NZ
1	A	212	LLP	C3-C4-C4'-NZ
1	H	212	LLP	C6-C5-C5'-OP4
1	H	212	LLP	C3-C4-C4'-NZ
1	G	212	LLP	CG-CD-CE-NZ
1	B	212	LLP	C5-C4-C4'-NZ
1	A	212	LLP	N-CA-CB-CG
1	H	212	LLP	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	212	LLP	2	0
1	A	212	LLP	2	0
1	F	212	LLP	3	0
1	H	212	LLP	4	0
1	B	212	LLP	2	0
1	D	212	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	$\# Z  > 2$
5	LPI	C	501	2	21,24,24	0.78	0	25,33,33	1.61	4 (16%)
6	CYS	F	501	-	3,6,6	0.32	0	1,7,7	0.03	0
4	SO4	B	501	1	4,4,4	0.12	0	6,6,6	0.29	0
4	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.07	0
6	CYS	H	501	-	3,6,6	0.46	0	1,7,7	0.48	0
3	MET	A	501	-	4,8,8	0.14	0	2,9,9	0.17	0
4	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.07	0
5	LPI	E	501	-	21,24,24	0.75	0	25,33,33	1.27	4 (16%)
6	CYS	G	501	-	3,6,6	0.32	0	1,7,7	0.02	0

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
5	LPI	C	501	2	-	6/15/19/19	0/1/1/1
6	CYS	F	501	-	-	0/2/6/6	-
6	CYS	H	501	-	-	2/2/6/6	-
3	MET	A	501	-	-	0/4/8/8	-
5	LPI	E	501	-	-	9/15/19/19	0/1/1/1
6	CYS	G	501	-	-	0/2/6/6	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	LPI	C4'-C4-C5	5.36	125.67	119.71
5	E	501	LPI	C6-C5-C4	3.07	120.29	118.12
5	E	501	LPI	C11-S10-C9	3.06	110.92	100.40
5	C	501	LPI	C4'-C4-C3	-2.44	117.43	120.04
5	C	501	LPI	C6-C5-C4	2.35	119.78	118.12
5	E	501	LPI	C4'-N3-C1	-2.26	109.49	113.83
5	E	501	LPI	C5-C6-N1	-2.26	120.05	123.82
5	C	501	LPI	C11-S10-C9	2.17	107.86	100.40

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	LPI	C7-C1-C8-C9
5	C	501	LPI	N3-C1-C8-C9
6	H	501	CYS	C-CA-CB-SG
5	E	501	LPI	C5'-OP4-P-OP1
5	E	501	LPI	C5'-OP4-P-OP3
5	E	501	LPI	C7-C1-C8-C9
5	E	501	LPI	N3-C1-C8-C9
5	E	501	LPI	C7-C1-N3-C4'
5	E	501	LPI	C1-C8-C9-S10
5	E	501	LPI	C8-C9-S10-C11
5	E	501	LPI	C8-C1-N3-C4'
5	C	501	LPI	C7-C1-N3-C4'
5	C	501	LPI	C4-C5-C5'-OP4
5	C	501	LPI	C8-C1-N3-C4'
5	C	501	LPI	C1-C8-C9-S10
6	H	501	CYS	N-CA-CB-SG
5	E	501	LPI	C5'-OP4-P-OP2

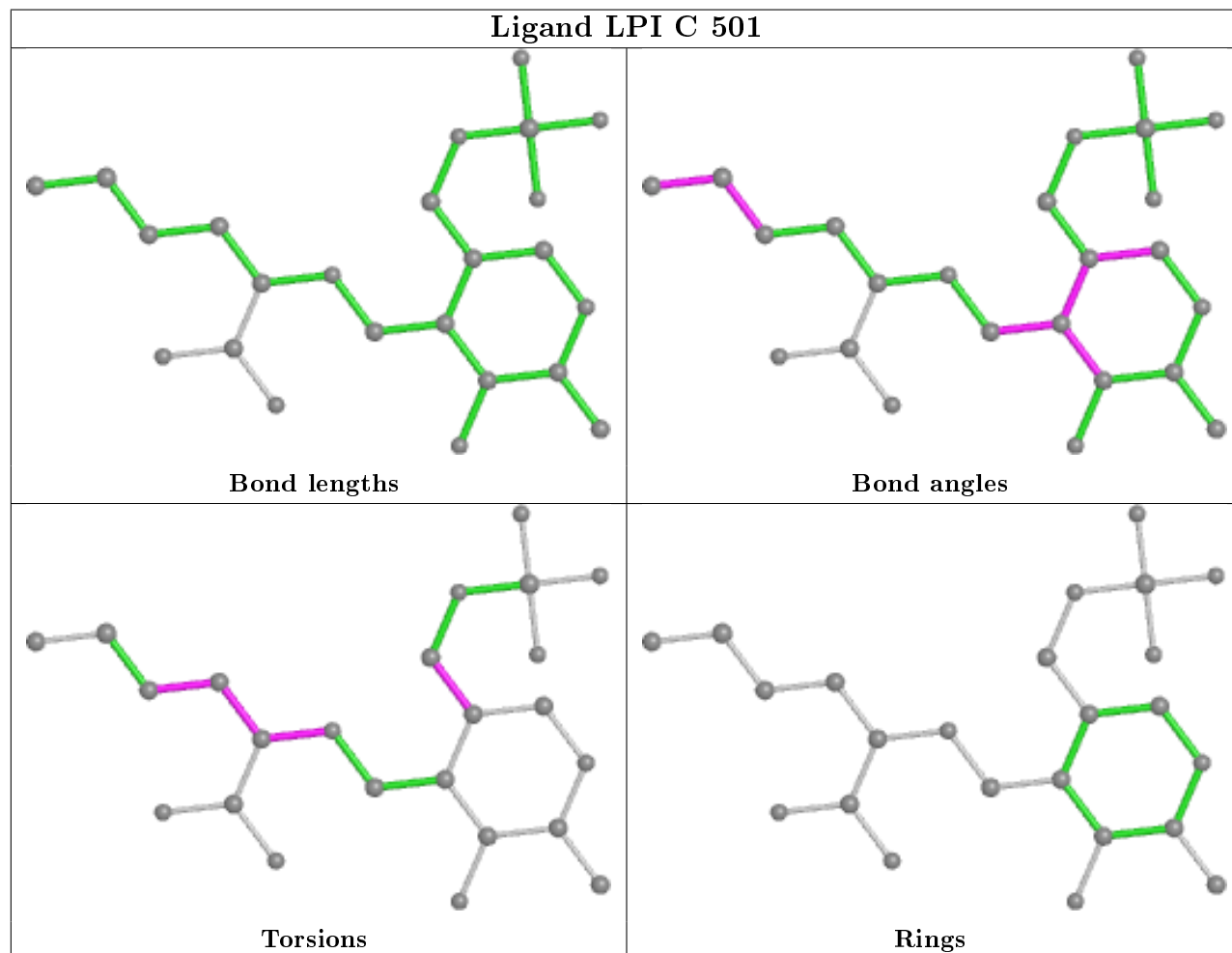
There are no ring outliers.

4 monomers are involved in 9 short contacts:

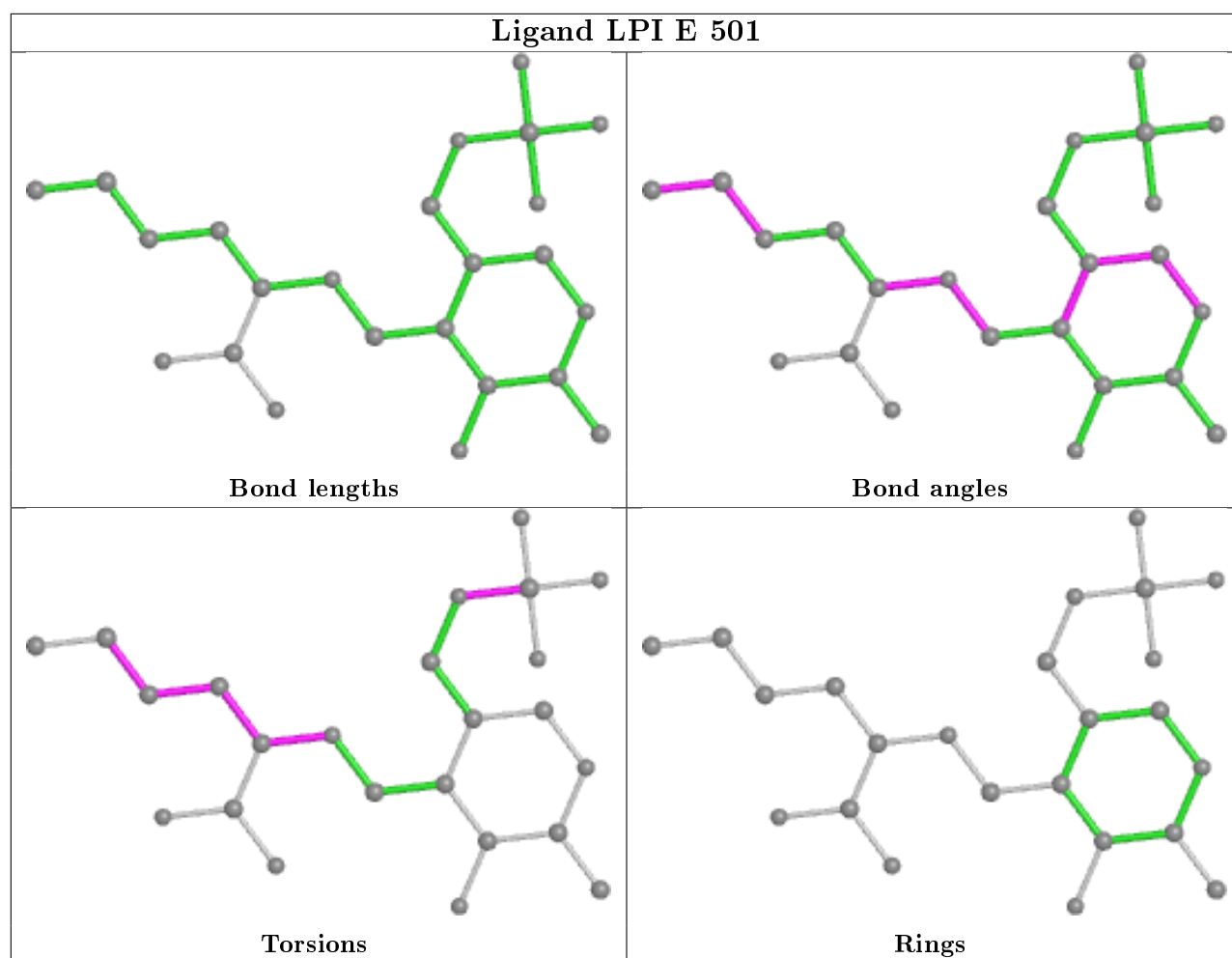
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	501	CYS	1	0
6	H	501	CYS	3	0
3	A	501	MET	2	0
5	E	501	LPI	3	0

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	383/422 (90%)	-0.25	10 (2%) 56 53	23, 35, 67, 102	0
1	B	384/422 (90%)	0.02	22 (5%) 23 22	25, 46, 84, 114	0
1	D	383/422 (90%)	0.09	24 (6%) 20 19	23, 43, 85, 114	0
1	F	380/422 (90%)	0.43	32 (8%) 11 9	41, 66, 108, 140	0
1	G	385/422 (91%)	0.38	31 (8%) 12 10	32, 60, 97, 122	0
1	H	385/422 (91%)	-0.14	11 (2%) 51 49	29, 50, 91, 109	0
2	C	386/422 (91%)	-0.28	10 (2%) 56 53	23, 36, 64, 88	0
2	E	385/422 (91%)	-0.05	10 (2%) 56 53	30, 53, 86, 102	0
All	All	3071/3376 (90%)	0.02	150 (4%) 29 28	23, 48, 91, 140	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	PRO	6.8
1	H	140	ILE	6.7
1	F	141	LYS	6.4
1	B	141	LYS	6.0
1	D	358	SER	5.1
1	A	362	ASN	5.0
1	D	367	LEU	5.0
1	D	366	VAL	4.9
1	G	362	ASN	4.8
1	F	399	PRO	4.7
1	G	400	PRO	4.7
1	D	357	ALA	4.5
1	F	146	ALA	4.4
1	G	360	LEU	4.3
1	G	254	LEU	4.3
1	F	179	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	325	ALA	4.2
1	D	356	HIS	4.1
1	F	13	PRO	4.1
1	B	179	HIS	4.1
1	H	359	VAL	4.0
1	B	322	LEU	4.0
1	B	397	ALA	4.0
1	F	356	HIS	4.0
2	E	179	HIS	3.9
1	F	311	THR	3.8
1	G	399	PRO	3.8
1	H	250	ILE	3.8
1	D	311	THR	3.7
1	B	325	ALA	3.6
1	F	250	ILE	3.6
1	F	142	LEU	3.5
1	D	365	ASP	3.5
1	G	250	ILE	3.5
1	D	399	PRO	3.5
1	F	366	VAL	3.4
1	A	50	GLY	3.4
2	E	145	ALA	3.3
2	C	250	ILE	3.3
1	D	364	ARG	3.3
2	C	56	SER	3.3
1	B	250	ILE	3.3
1	F	295	PRO	3.3
1	B	142	LEU	3.2
1	D	397	ALA	3.2
1	D	250	ILE	3.2
1	A	250	ILE	3.2
1	G	179	HIS	3.2
1	G	178	LYS	3.2
1	G	356	HIS	3.2
1	F	357	ALA	3.1
1	B	396	ALA	3.1
2	C	311	THR	3.1
1	B	178	LYS	3.1
1	G	252	CYS	3.1
1	H	56	SER	3.0
1	A	311	THR	3.0
1	D	220	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	394	LEU	3.0
1	F	112	ASP	3.0
1	H	311	THR	3.0
1	F	140	ILE	2.9
1	H	154	VAL	2.9
1	H	360	LEU	2.9
2	E	250	ILE	2.8
1	B	285	TRP	2.8
1	H	367	LEU	2.8
1	B	220	VAL	2.8
1	B	56	SER	2.8
1	D	369	ILE	2.8
2	E	254	LEU	2.8
1	D	353	ILE	2.8
1	G	253	TYR	2.7
1	D	111	ASP	2.7
1	D	112	ASP	2.7
1	F	285	TRP	2.7
1	G	366	VAL	2.7
1	D	322	LEU	2.7
1	B	353	ILE	2.6
1	B	311	THR	2.6
1	B	366	VAL	2.6
1	G	149	PRO	2.6
1	G	323	GLN	2.6
1	F	369	ILE	2.6
1	H	141	LYS	2.6
1	G	311	THR	2.6
2	E	311	THR	2.6
1	G	150	GLU	2.6
1	H	254	LEU	2.5
1	F	50	GLY	2.5
1	B	352	ALA	2.5
1	G	322	LEU	2.5
1	A	358	SER	2.5
1	F	51	ALA	2.5
1	G	321	THR	2.5
1	F	144	GLU	2.5
1	F	178	LYS	2.4
1	D	323	GLN	2.4
1	D	56	SER	2.4
1	G	251	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	252	CYS	2.4
1	G	248	SER	2.4
1	F	169	ILE	2.4
2	C	88	ALA	2.4
1	B	254	LEU	2.4
2	E	252	CYS	2.4
1	F	83	TYR	2.3
1	D	51	ALA	2.3
2	C	248	SER	2.3
1	H	358	SER	2.3
1	F	57	GLY	2.3
2	E	248	SER	2.3
1	D	354	MET	2.3
2	C	222	MET	2.3
1	F	248	SER	2.3
1	G	289	VAL	2.2
1	D	396	ALA	2.2
1	D	258	GLY	2.2
1	F	180	GLY	2.2
1	F	134	PHE	2.2
1	A	248	SER	2.2
1	G	56	SER	2.2
1	G	211	THR	2.2
1	B	324	HIS	2.2
1	G	258	GLY	2.2
1	A	141	LYS	2.2
1	F	221	VAL	2.2
1	F	397	ALA	2.2
1	G	353	ILE	2.1
1	F	367	LEU	2.1
1	G	367	LEU	2.1
2	E	249	PRO	2.1
1	G	257	ARG	2.1
1	A	254	LEU	2.1
1	D	52	PRO	2.1
1	G	315	THR	2.1
1	B	10	GLY	2.1
2	C	249	PRO	2.1
1	A	363	ASP	2.1
2	C	255	CYS	2.1
1	A	179	HIS	2.1
1	B	367	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	253	TYR	2.1
1	G	12	LEU	2.0
1	F	355	THR	2.0
1	F	16	GLN	2.0
2	E	400	PRO	2.0
1	B	398	HIS	2.0
2	C	254	LEU	2.0
1	F	365	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	G	212	24/25	0.95	0.16	43,51,61,65	0
1	LLP	F	212	24/25	0.95	0.15	46,56,62,63	0
1	LLP	B	212	24/25	0.95	0.14	35,42,51,63	0
1	LLP	H	212	24/25	0.96	0.14	34,43,50,54	0
1	LLP	D	212	24/25	0.96	0.14	31,39,48,52	0
1	LLP	A	212	24/25	0.97	0.16	22,30,34,37	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	501	5/5	0.64	0.35	34,37,43,52	5
6	CYS	G	501	7/7	0.76	0.29	64,71,88,89	0
6	CYS	F	501	7/7	0.80	0.24	72,72,83,87	0
3	MET	A	501	9/9	0.87	0.27	41,64,85,87	0

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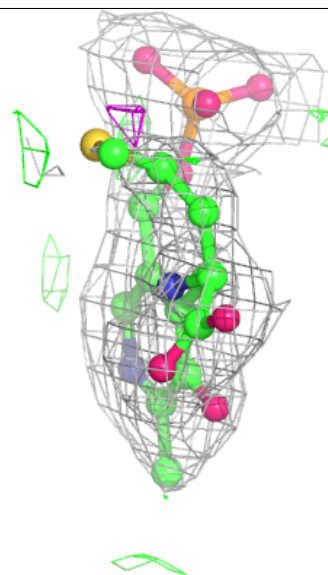
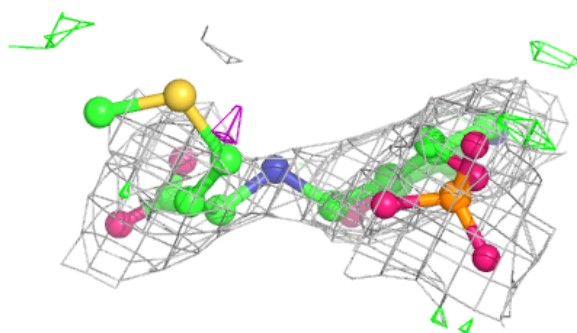
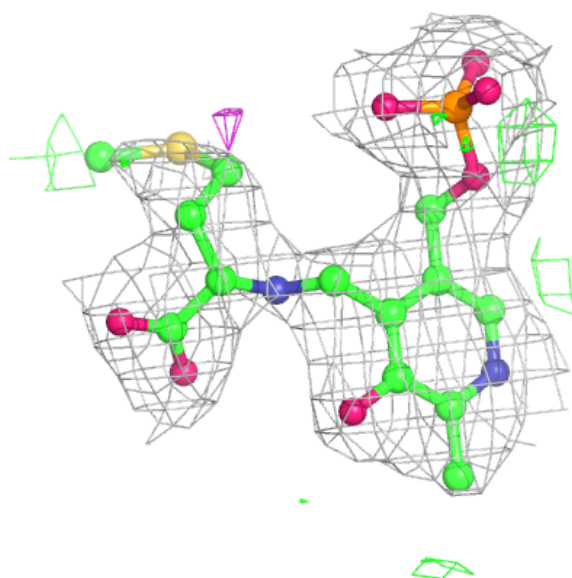
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	502	5/5	0.89	0.17	109,110,110,112	0
6	CYS	H	501	7/7	0.89	0.17	48,53,72,81	0
5	LPI	E	501	24/24	0.95	0.12	39,49,53,58	3
5	LPI	C	501	24/24	0.95	0.17	23,35,64,80	0
4	SO4	D	501	5/5	0.98	0.09	62,64,73,73	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.

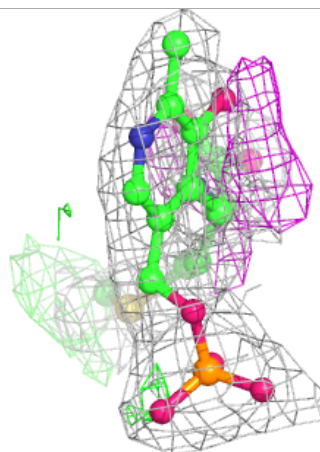
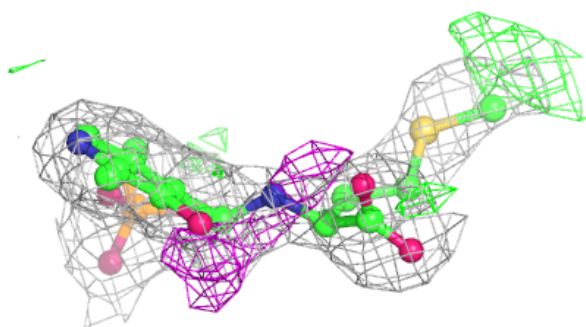
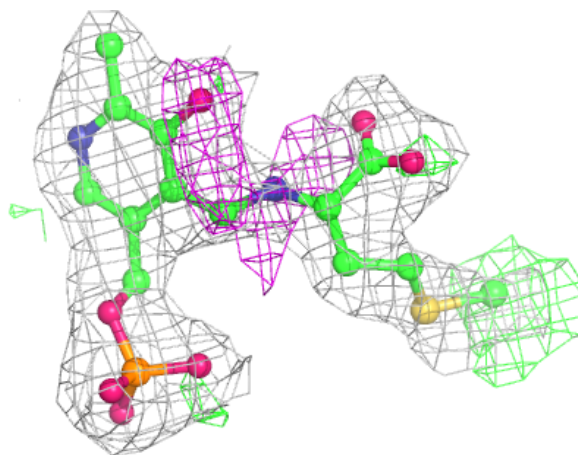
**Electron density around LPI E 501:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LPI 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.