



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 05:27 AM EDT

PDB ID : 6SMW
Title : A. thaliana serine hydroxymethyltransferase isoform 2 (AtSHMT2) in complex with pemetrexed
Authors : Ruszkowski, M.; Sekula, B.; Dauter, Z.
Deposited on : 2019-08-23
Resolution : 1.54 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

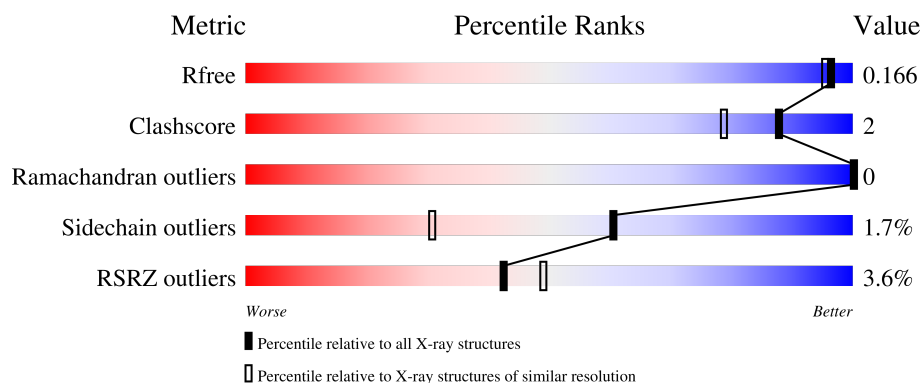
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	480	<div> <div>3%</div> <div>95%</div> <div>5%</div> <div>5%</div> </div>
1	B	480	<div> <div>4%</div> <div>95%</div> <div>5%</div> <div>5%</div> </div>
1	C	480	<div> <div>2%</div> <div>94%</div> <div>5%</div> <div>5%</div> </div>
1	D	480	<div> <div>5%</div> <div>95%</div> <div>5%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	C	614	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17445 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.

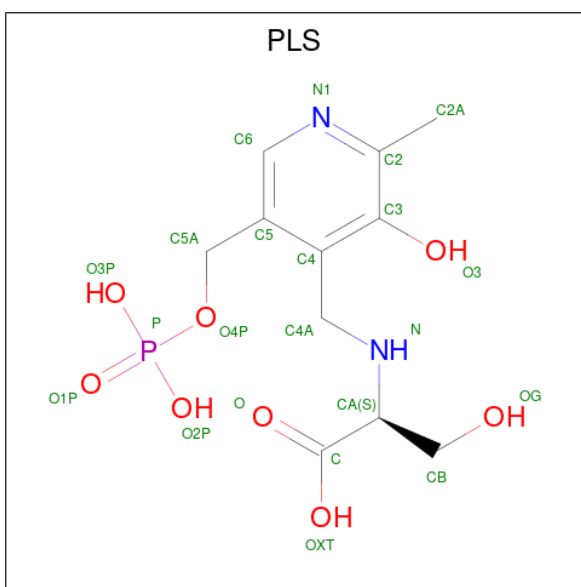
- Molecule 1 is a protein called Serine hydroxymethyltransferase 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	7	0
			3786	2404	647	716	19			
1	B	475	Total	C	N	O	S	0	4	0
			3755	2382	643	712	18			
1	C	475	Total	C	N	O	S	0	11	0
			3804	2408	653	725	18			
1	D	480	Total	C	N	O	S	0	7	0
			3831	2430	658	724	19			

There are 12 discrepancies between the modelled and reference sequences:

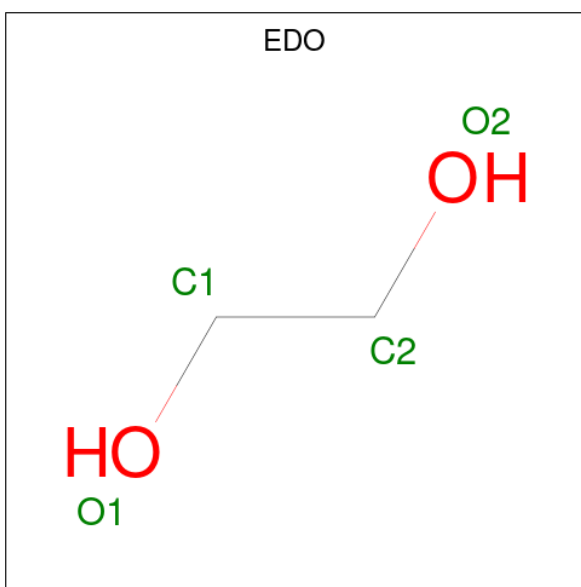
Chain	Residue	Modelled	Actual	Comment	Reference
A	38	SER	-	expression tag	UNP Q94C74
A	39	ASN	-	expression tag	UNP Q94C74
A	40	ALA	-	expression tag	UNP Q94C74
B	38	SER	-	expression tag	UNP Q94C74
B	39	ASN	-	expression tag	UNP Q94C74
B	40	ALA	-	expression tag	UNP Q94C74
C	38	SER	-	expression tag	UNP Q94C74
C	39	ASN	-	expression tag	UNP Q94C74
C	40	ALA	-	expression tag	UNP Q94C74
D	38	SER	-	expression tag	UNP Q94C74
D	39	ASN	-	expression tag	UNP Q94C74
D	40	ALA	-	expression tag	UNP Q94C74

- Molecule 2 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: C₁₁H₁₇N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 22	C 11	N 2	O 8	P 1	0	0
2	B	1	Total 22	C 11	N 2	O 8	P 1	0	0
2	C	1	Total 22	C 11	N 2	O 8	P 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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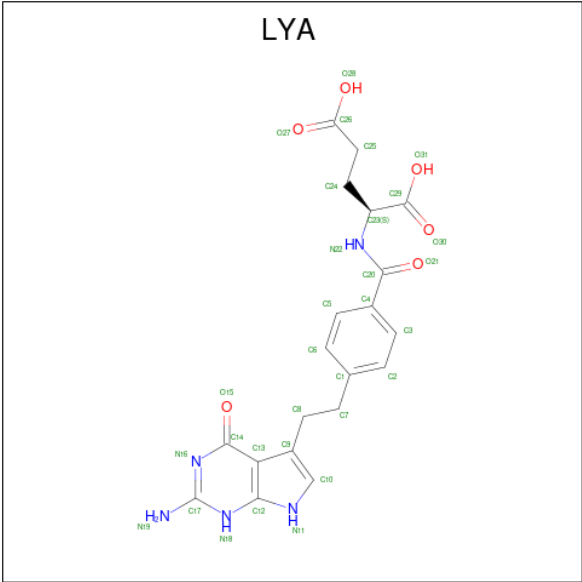
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

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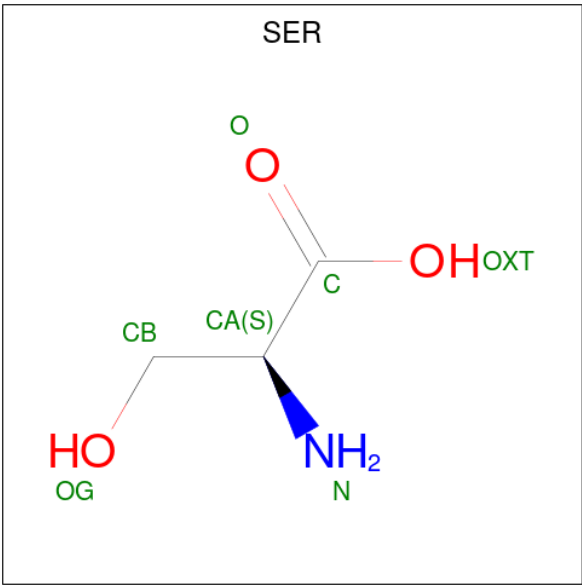
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is 2-{4-[2-(2-AMINO-4-OXO-4,7-DIHYDRO-3H-PYRROLO[2,3-D]PYRIMIDIN-5-YL)-ETHYL]-BENZOYLAMINO}-PENTANEDIOIC ACID (three-letter code: LYA) (formula: C₂₀H₂₁N₅O₆) (labeled as "Ligand of Interest" by depositor).



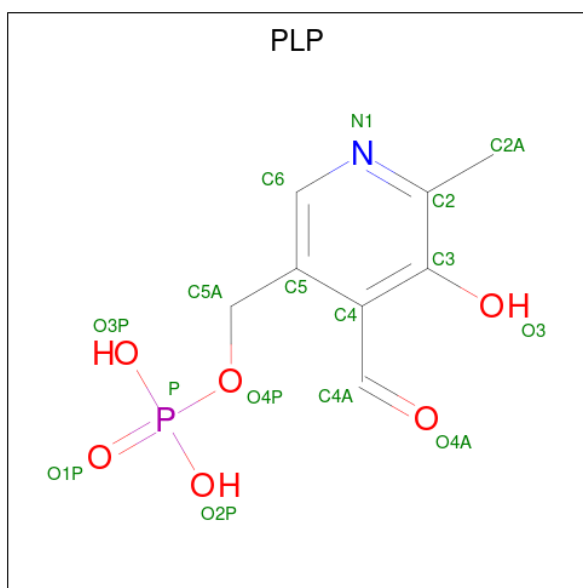
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			31	20	5	6		
4	C	1	Total	C	N	O	0	0
			31	20	5	6		
4	D	1	Total	C	N	O	0	0
			31	20	5	6		

- Molecule 5 is SERINE (three-letter code: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

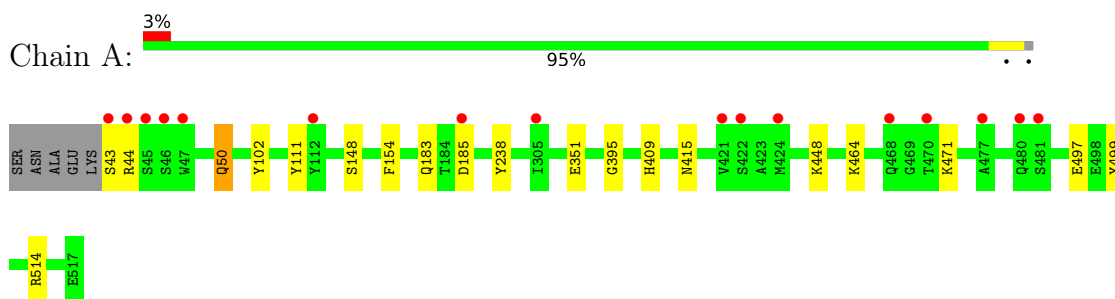
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	503	Total	O	0	0
			503	503		
7	B	450	Total	O	0	0
			450	450		
7	C	528	Total	O	0	0
			528	528		
7	D	455	Total	O	0	0
			455	455		

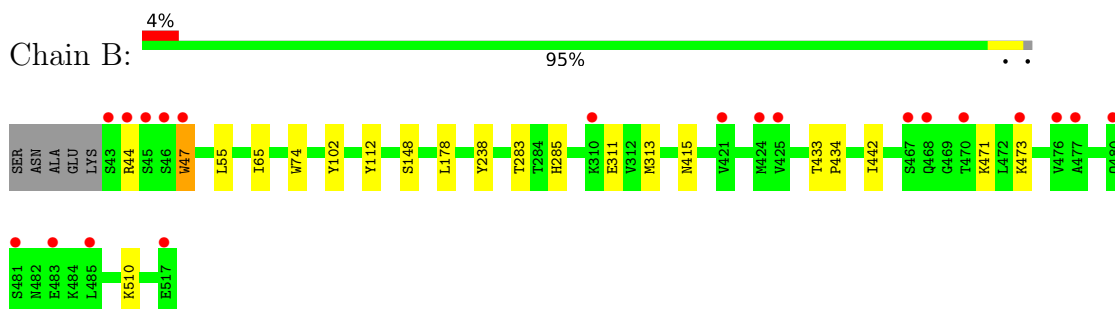
3 Residue-property plots [i](#)

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.

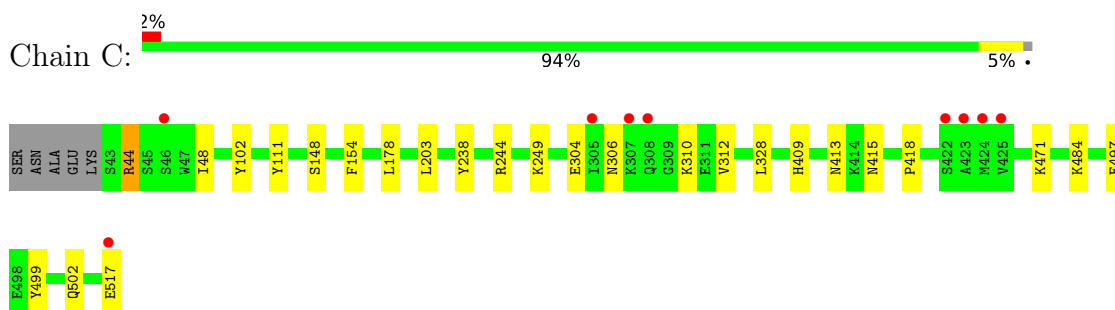
- Molecule 1: Serine hydroxymethyltransferase 2, mitochondrial



- Molecule 1: Serine hydroxymethyltransferase 2, mitochondrial

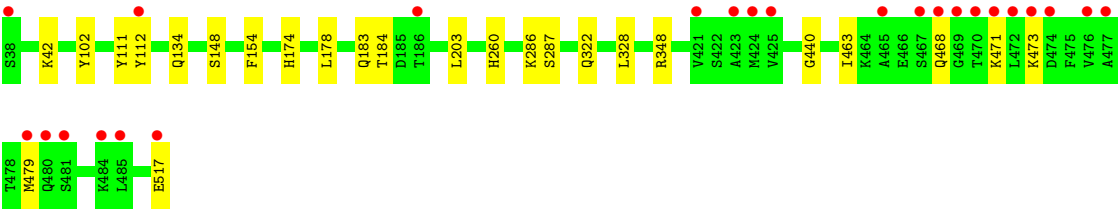


- Molecule 1: Serine hydroxymethyltransferase 2, mitochondrial



- Molecule 1: Serine hydroxymethyltransferase 2, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.90Å 130.29Å 150.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 1.54 75.39 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (80.00-1.54) 99.7 (75.39-1.54)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.129 , 0.166 0.129 , 0.166	Depositor DCC
R_{free} test set	1321 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	17445	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, LYA, PLP, PLS

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	0.33	0/3862	0.51	0/5209
1	B	0.32	0/3830	0.51	0/5167
1	C	0.34	0/3879	0.52	0/5232
1	D	0.32	0/3907	0.51	0/5268
All	All	0.33	0/15478	0.51	0/20876

There are no bond length outliers.

There are no bond angle outliers.

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	3786	0	3783	14	0
1	B	3755	0	3751	14	0
1	C	3804	0	3791	16	0
1	D	3831	0	3827	16	0
2	A	22	0	14	1	0
2	B	22	0	14	2	0
2	C	22	0	14	1	0
3	A	36	0	54	1	0
3	B	36	0	54	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	48	0	72	6	0
3	D	32	0	48	1	0
4	A	31	0	19	4	0
4	C	31	0	19	5	0
4	D	31	0	19	3	0
5	C	7	0	4	1	0
6	D	15	0	7	1	0
7	A	503	0	0	6	0
7	B	450	0	0	0	0
7	C	528	0	0	3	0
7	D	455	0	0	5	0
All	All	17445	0	15490	62	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 2.

All (62) 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:50:GLN:NE2	7:A:802:HOH:O	2.31	0.63
1:C:471:LYS:HB3	3:C:605:EDO:H12	1.80	0.63
4:C:608:LYA:N18	7:C:705:HOH:O	2.31	0.62
1:A:395:GLY:O	1:A:464:LYS:NZ	2.34	0.60
1:A:154:PHE:CD1	3:A:703:EDO:H22	2.36	0.60
4:A:710:LYA:HC72	1:B:178:LEU:HD11	1.85	0.59
2:C:601:PLS:HB1	7:D:1427:HOH:O	2.06	0.56
7:A:910:HOH:O	2:B:601:PLS:HB1	2.05	0.55
1:C:409[B]:HIS:ND1	1:C:497:GLU:OE2	2.39	0.55
1:A:183:GLN:NE2	7:A:805:HOH:O	2.32	0.55
1:A:185:ASP:HB2	7:D:1724:HOH:O	2.07	0.54
1:C:244:ARG:NH2	7:C:704:HOH:O	2.31	0.54
2:A:701:PLS:HB2	1:B:112:TYR:OH	2.08	0.54
4:C:608:LYA:HC81	1:D:111[B]:TYR:CE1	2.45	0.52
1:C:44:ARG:HD3	1:D:440:GLY:O	2.09	0.52
1:D:286:LYS:NZ	6:D:1310:PLP:O3	2.42	0.51
1:C:328:LEU:HD22	3:C:614:EDO:H22	1.92	0.50
1:C:44:ARG:O	1:C:48:ILE:HG12	2.12	0.50
3:C:615:EDO:H21	1:D:322:GLN:HB3	1.95	0.49
1:C:413:ASN:CB	1:D:112[B]:TYR:HB3	2.42	0.49
1:D:471:LYS:HA	1:D:471:LYS:HD2	1.65	0.49
1:C:154:PHE:CD1	3:C:614:EDO:H12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:613:SER:N	4:D:1305:LYA:H18	2.11	0.48
1:A:514:ARG:NH1	7:A:810:HOH:O	2.46	0.47
1:C:306:ASN:HD21	1:C:310:LYS:HB2	1.79	0.47
1:C:111:TYR:CE2	4:D:1305:LYA:HC82	2.49	0.47
7:C:869:HOH:O	3:D:1301:EDO:H11	2.13	0.47
1:A:44:ARG:NH1	7:A:809:HOH:O	2.46	0.47
1:A:111[B]:TYR:CE1	4:A:710:LYA:HC81	2.50	0.46
1:D:42:LYS:NZ	7:D:1412:HOH:O	2.48	0.46
1:C:304:GLU:HG2	1:C:312:VAL:CG1	2.45	0.46
3:C:614:EDO:H11	1:D:328:LEU:HD22	1.97	0.46
1:C:178:LEU:HD11	4:C:608:LYA:C7	2.45	0.46
1:C:203:LEU:HD12	1:C:418:PRO:HG3	1.98	0.46
4:C:608:LYA:HC81	1:D:111[A]:TYR:CE2	2.51	0.46
1:A:111[A]:TYR:CE2	4:A:710:LYA:HC81	2.51	0.45
1:B:55:LEU:HD23	3:B:609:EDO:H11	1.98	0.45
7:A:910:HOH:O	2:B:601:PLS:H4A2	2.16	0.45
1:D:178:LEU:HD11	4:D:1305:LYA:HC71	1.98	0.45
3:C:614:EDO:H21	1:D:154:PHE:CD1	2.52	0.45
1:A:351:GLU:HB3	1:B:47:TRP:HB3	1.99	0.45
1:A:471:LYS:HD2	1:A:471:LYS:HA	1.84	0.44
1:B:471:LYS:HA	1:B:471:LYS:HD2	1.71	0.44
1:B:311:GLU:HG3	1:B:313:MET:H	1.83	0.44
1:A:44:ARG:HD3	1:B:442:ILE:HG23	2.00	0.44
1:C:178:LEU:HD11	4:C:608:LYA:HC72	2.00	0.44
1:D:174:HIS:HB3	1:D:203:LEU:HG	2.00	0.44
1:C:499:TYR:O	1:C:502:GLN:HG2	2.18	0.44
1:D:183[B]:GLN:HG2	1:D:184:THR:O	2.18	0.43
1:D:112[B]:TYR:HA	7:D:1634:HOH:O	2.18	0.43
1:B:74:TRP:NE1	1:B:510:LYS:HE2	2.34	0.43
1:C:306:ASN:ND2	1:C:310:LYS:HB2	2.34	0.43
1:D:348[A]:ARG:HG2	7:D:1467:HOH:O	2.19	0.42
1:B:65:ILE:HG13	3:B:605:EDO:H11	2.01	0.42
1:A:409:HIS:ND1	1:A:497:GLU:OE2	2.52	0.42
4:A:710:LYA:C7	1:B:178:LEU:HD11	2.50	0.41
1:B:283:THR:HB	1:B:285:HIS:CE1	2.56	0.41
1:D:463:ILE:HD13	1:D:479:MET:HG3	2.03	0.41
1:B:473:LYS:HA	1:B:473:LYS:HE2	2.02	0.40
1:A:448:LYS:HG2	1:A:499:TYR:CE2	2.56	0.40
1:B:44:ARG:HA	1:B:47:TRP:CE3	2.57	0.40
1:B:433:THR:N	1:B:434:PRO:CD	2.85	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	480/480 (100%)	466 (97%)	14 (3%)	0	100	100
1	B	477/480 (99%)	465 (98%)	12 (2%)	0	100	100
1	C	484/480 (101%)	471 (97%)	13 (3%)	0	100	100
1	D	485/480 (101%)	473 (98%)	12 (2%)	0	100	100
All	All	1926/1920 (100%)	1875 (97%)	51 (3%)	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	404/401 (101%)	398 (98%)	6 (2%)	65	36
1	B	401/401 (100%)	396 (99%)	5 (1%)	71	47
1	C	408/401 (102%)	400 (98%)	8 (2%)	55	24
1	D	408/401 (102%)	400 (98%)	8 (2%)	55	24
All	All	1621/1604 (101%)	1594 (98%)	27 (2%)	60	31

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	50	GLN

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Mol	Chain	Res	Type
1	A	102	TYR
1	A	148	SER
1	A	238	TYR
1	A	415	ASN
1	B	47	TRP
1	B	102	TYR
1	B	148	SER
1	B	238	TYR
1	B	415	ASN
1	C	44	ARG
1	C	102	TYR
1	C	148	SER
1	C	238	TYR
1	C	249	LYS
1	C	415	ASN
1	C	484	LYS
1	C	517	GLU
1	D	102	TYR
1	D	134	GLN
1	D	148	SER
1	D	260	HIS
1	D	287	SER
1	D	468	GLN
1	D	473	LYS
1	D	517	GLU

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

Mol	Chain	Res	Type
1	A	308	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

46 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	$\# Z > 2$
3	EDO	B	610	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	C	611	-	3,3,3	0.45	0	2,2,2	0.44	0
3	EDO	B	603	-	3,3,3	0.43	0	2,2,2	0.58	0
3	EDO	B	602	-	3,3,3	0.43	0	2,2,2	0.52	0
3	EDO	B	608	-	3,3,3	0.51	0	2,2,2	0.26	0
3	EDO	B	609	-	3,3,3	0.34	0	2,2,2	0.59	0
3	EDO	C	602	-	3,3,3	0.32	0	2,2,2	0.65	0
3	EDO	D	1301	-	3,3,3	0.49	0	2,2,2	0.30	0
3	EDO	C	612	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	B	605	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	A	707	-	3,3,3	0.43	0	2,2,2	0.48	0
3	EDO	C	603	-	3,3,3	0.42	0	2,2,2	0.43	0
5	SER	C	613	-	5,6,6	0.98	1 (20%)	5,7,7	1.54	2 (40%)
3	EDO	C	610	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	A	702	-	3,3,3	0.41	0	2,2,2	0.51	0
3	EDO	D	1309	-	3,3,3	0.45	0	2,2,2	0.50	0
3	EDO	B	607	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	A	708	-	3,3,3	0.43	0	2,2,2	0.43	0
2	PLS	B	601	-	22,22,22	1.83	2 (9%)	27,31,31	1.59	5 (18%)
3	EDO	C	607	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	D	1303	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	C	615	-	3,3,3	0.44	0	2,2,2	0.47	0
6	PLP	D	1310	1	15,15,16	2.13	5 (33%)	20,22,23	1.67	2 (10%)
2	PLS	A	701	-	22,22,22	1.91	3 (13%)	27,31,31	1.53	5 (18%)
3	EDO	C	606	-	3,3,3	0.52	0	2,2,2	0.27	0
3	EDO	B	604	-	3,3,3	0.43	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	614	-	3,3,3	0.35	0	2,2,2	0.63	0
4	LYA	A	710	-	32,33,33	1.57	2 (6%)	35,46,46	2.05	2 (5%)
3	EDO	A	705	-	3,3,3	0.48	0	2,2,2	0.32	0
4	LYA	D	1305	-	32,33,33	1.50	4 (12%)	35,46,46	2.02	2 (5%)
3	EDO	D	1308	-	3,3,3	0.47	0	2,2,2	0.35	0
3	EDO	A	703	-	3,3,3	0.34	0	2,2,2	0.49	0
3	EDO	B	606	-	3,3,3	0.46	0	2,2,2	0.29	0
3	EDO	D	1307	-	3,3,3	0.47	0	2,2,2	0.37	0
3	EDO	D	1302	-	3,3,3	0.43	0	2,2,2	0.46	0
3	EDO	C	605	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	D	1304	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	A	711	-	3,3,3	0.46	0	2,2,2	0.38	0
2	PLS	C	601	-	22,22,22	1.92	3 (13%)	27,31,31	1.59	4 (14%)
3	EDO	A	706	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	D	1306	-	3,3,3	0.46	0	2,2,2	0.40	0
3	EDO	A	709	-	3,3,3	0.45	0	2,2,2	0.46	0
4	LYA	C	608	-	32,33,33	1.54	2 (6%)	35,46,46	2.15	2 (5%)
3	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	C	609	-	3,3,3	0.43	0	2,2,2	0.42	0
3	EDO	C	604	-	3,3,3	0.45	0	2,2,2	0.49	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
3	EDO	B	610	-	-	0/1/1/1	-
3	EDO	C	611	-	-	0/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	B	602	-	-	0/1/1/1	-
3	EDO	B	608	-	-	1/1/1/1	-
3	EDO	B	609	-	-	0/1/1/1	-
3	EDO	C	602	-	-	1/1/1/1	-
3	EDO	D	1301	-	-	1/1/1/1	-
3	EDO	C	612	-	-	1/1/1/1	-
3	EDO	B	605	-	-	0/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	C	603	-	-	0/1/1/1	-
5	SER	C	613	-	-	2/6/6/6	-
3	EDO	C	610	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	D	1309	-	-	1/1/1/1	-
3	EDO	B	607	-	-	0/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
2	PLS	B	601	-	-	3/17/17/17	0/1/1/1
3	EDO	C	607	-	-	0/1/1/1	-
3	EDO	D	1303	-	-	0/1/1/1	-
3	EDO	C	615	-	-	0/1/1/1	-
6	PLP	D	1310	1	-	0/6/6/8	0/1/1/1
2	PLS	A	701	-	-	3/17/17/17	0/1/1/1
3	EDO	C	606	-	-	0/1/1/1	-
3	EDO	B	604	-	-	0/1/1/1	-
3	EDO	C	614	-	-	0/1/1/1	-
4	LYA	A	710	-	-	0/22/22/22	0/3/3/3
3	EDO	A	705	-	-	0/1/1/1	-
4	LYA	D	1305	-	-	0/22/22/22	0/3/3/3
3	EDO	D	1308	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	B	606	-	-	0/1/1/1	-
3	EDO	D	1307	-	-	0/1/1/1	-
3	EDO	D	1302	-	-	0/1/1/1	-
3	EDO	C	605	-	-	1/1/1/1	-
3	EDO	D	1304	-	-	0/1/1/1	-
3	EDO	A	711	-	-	0/1/1/1	-
2	PLS	C	601	-	-	3/17/17/17	0/1/1/1
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	D	1306	-	-	0/1/1/1	-
3	EDO	A	709	-	-	1/1/1/1	-
4	LYA	C	608	-	-	2/22/22/22	0/3/3/3
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	C	609	-	-	0/1/1/1	-
3	EDO	C	604	-	-	0/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PLS	C4A-N	-7.05	1.25	1.46
2	C	601	PLS	C4A-N	-6.94	1.26	1.46
2	B	601	PLS	C4A-N	-6.53	1.27	1.46
4	A	710	LYA	C14-N16	6.50	1.44	1.33
4	C	608	LYA	C14-N16	6.41	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1305	LYA	C14-N16	6.12	1.43	1.33
6	D	1310	PLP	C4A-C4	4.74	1.61	1.51
6	D	1310	PLP	C2A-C2	3.77	1.56	1.50
6	D	1310	PLP	C6-N1	2.72	1.40	1.34
4	A	710	LYA	C17-N19	2.52	1.39	1.33
4	D	1305	LYA	C17-N19	2.47	1.38	1.33
4	C	608	LYA	C17-N19	2.42	1.38	1.33
6	D	1310	PLP	C5A-C5	2.34	1.57	1.50
2	C	601	PLS	C5-C4	-2.34	1.37	1.40
6	D	1310	PLP	C5-C4	-2.30	1.38	1.40
2	A	701	PLS	C5-C4	-2.21	1.37	1.40
4	D	1305	LYA	C10-N11	2.13	1.41	1.36
5	C	613	SER	OXT-C	-2.11	1.23	1.30
2	B	601	PLS	C3-C2	-2.11	1.38	1.40
2	C	601	PLS	C3-C2	-2.06	1.38	1.40
2	A	701	PLS	C3-C4	-2.02	1.36	1.40
4	D	1305	LYA	C12-N11	2.01	1.38	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	608	LYA	C12-C13-C14	8.36	119.73	115.01
4	A	710	LYA	C12-C13-C14	7.82	119.42	115.01
4	D	1305	LYA	C12-C13-C14	7.72	119.37	115.01
4	C	608	LYA	C13-C14-N16	-7.46	117.47	124.09
4	A	710	LYA	C13-C14-N16	-7.33	117.58	124.09
4	D	1305	LYA	C13-C14-N16	-7.13	117.76	124.09
6	D	1310	PLP	O4P-C5A-C5	5.55	119.92	109.35
2	C	601	PLS	C4A-N-CA	4.39	122.24	113.92
2	B	601	PLS	C4A-N-CA	4.26	121.98	113.92
2	A	701	PLS	O4P-C5A-C5	4.11	117.17	109.35
2	B	601	PLS	O4P-C5A-C5	3.46	115.95	109.35
2	C	601	PLS	C4-C4A-N	3.31	120.90	111.78
2	C	601	PLS	O4P-C5A-C5	3.30	115.64	109.35
2	A	701	PLS	C4A-N-CA	3.29	120.15	113.92
2	B	601	PLS	C4-C4A-N	3.05	120.17	111.78
2	A	701	PLS	C4-C4A-N	2.51	118.69	111.78
5	C	613	SER	OXT-C-O	-2.38	118.67	124.09
2	B	601	PLS	C6-C5-C4	2.34	119.77	118.12
5	C	613	SER	OXT-C-CA	2.28	121.14	113.38
2	A	701	PLS	OXT-C-CA	2.26	120.92	113.40
6	D	1310	PLP	C5A-C5-C6	-2.21	115.73	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	PLS	C5-C6-N1	-2.15	120.24	123.82
2	A	701	PLS	C6-C5-C4	2.11	119.61	118.12
2	C	601	PLS	C6-C5-C4	2.01	119.54	118.12

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	PLS	C5-C4-C4A-N
2	B	601	PLS	C-CA-N-C4A
2	B	601	PLS	C3-C4-C4A-N
2	B	601	PLS	C5-C4-C4A-N
2	C	601	PLS	C-CA-N-C4A
2	C	601	PLS	C3-C4-C4A-N
2	C	601	PLS	C5-C4-C4A-N
3	A	709	EDO	O1-C1-C2-O2
3	D	1301	EDO	O1-C1-C2-O2
3	C	605	EDO	O1-C1-C2-O2
4	C	608	LYA	C29-C23-C24-C25
2	A	701	PLS	C-CA-N-C4A
3	C	612	EDO	O1-C1-C2-O2
4	C	608	LYA	N22-C23-C24-C25
2	A	701	PLS	C3-C4-C4A-N
5	C	613	SER	O-C-CA-N
3	C	602	EDO	O1-C1-C2-O2
3	B	608	EDO	O1-C1-C2-O2
5	C	613	SER	OXT-C-CA-CB
3	D	1309	EDO	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 27 short contacts:

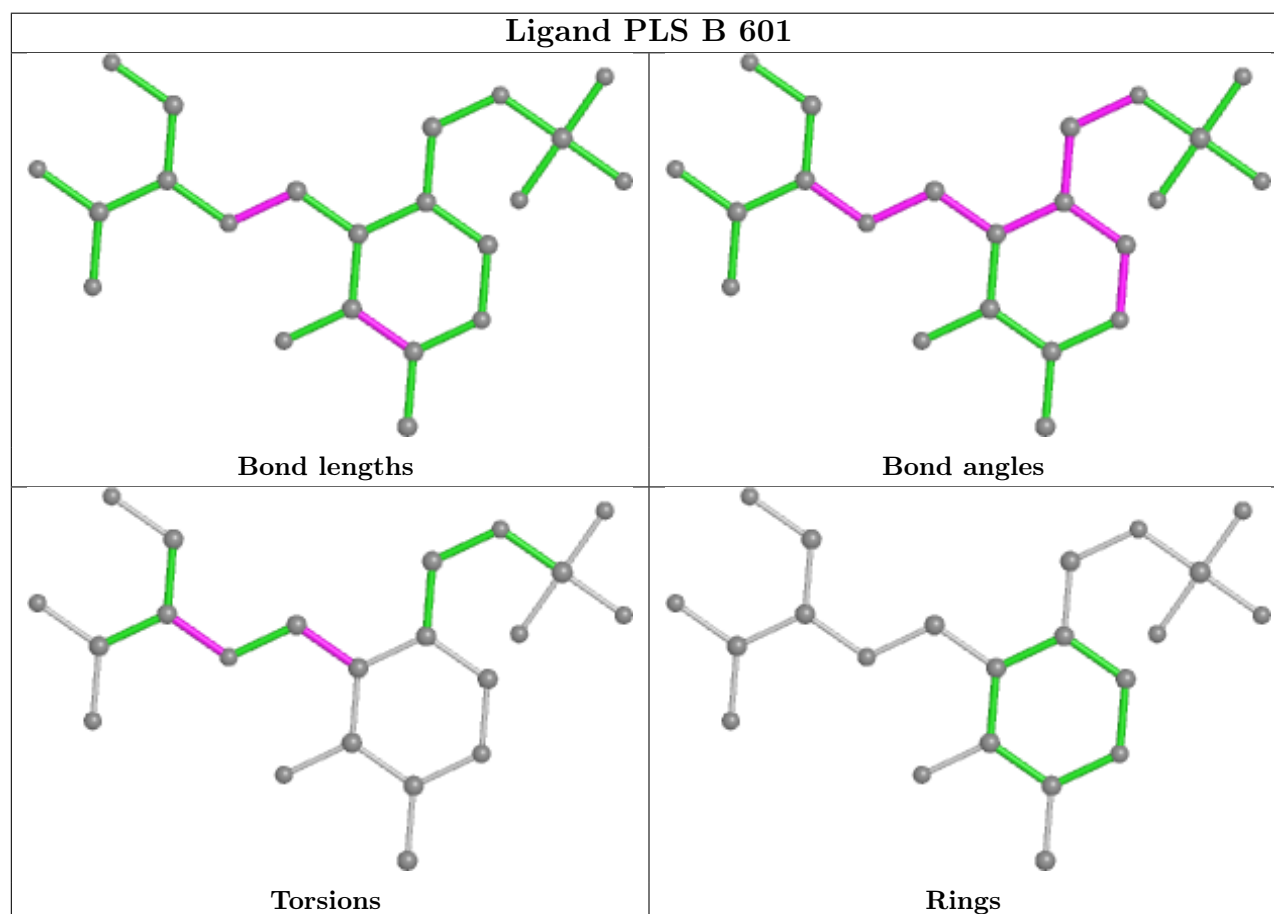
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	609	EDO	1	0
3	D	1301	EDO	1	0
3	B	605	EDO	1	0
5	C	613	SER	1	0
2	B	601	PLS	2	0
3	C	615	EDO	1	0
6	D	1310	PLP	1	0
2	A	701	PLS	1	0

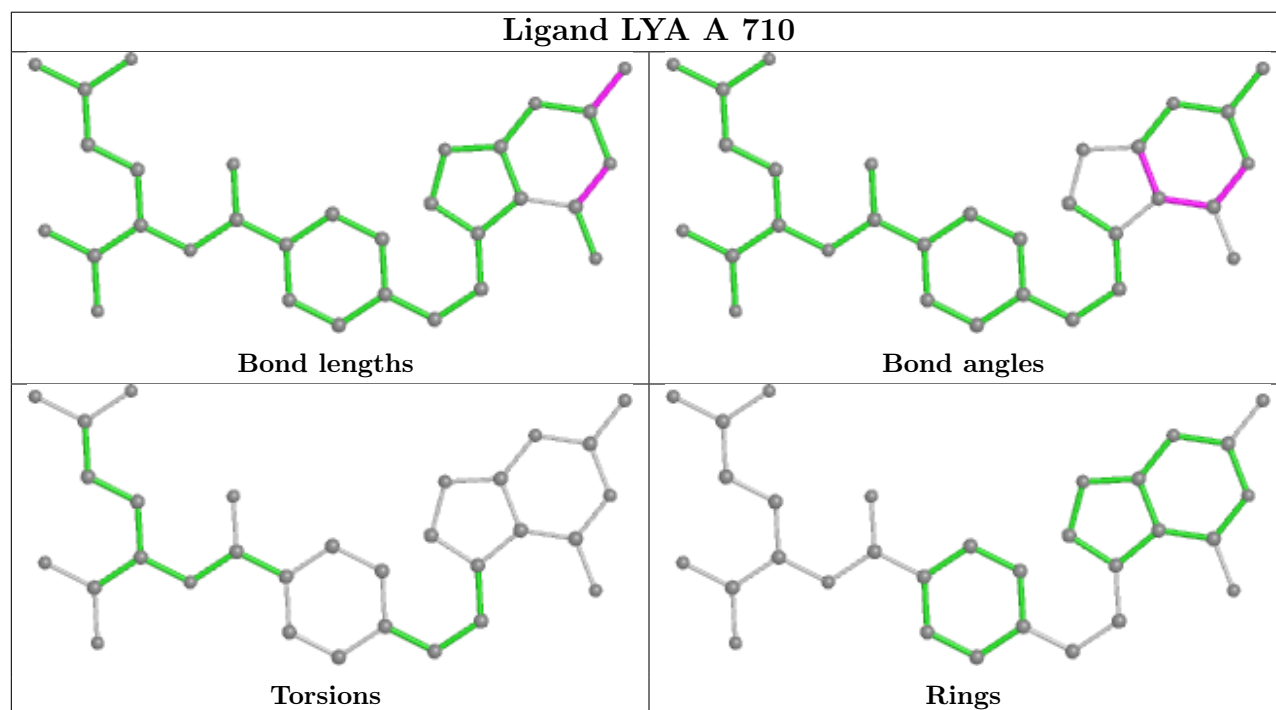
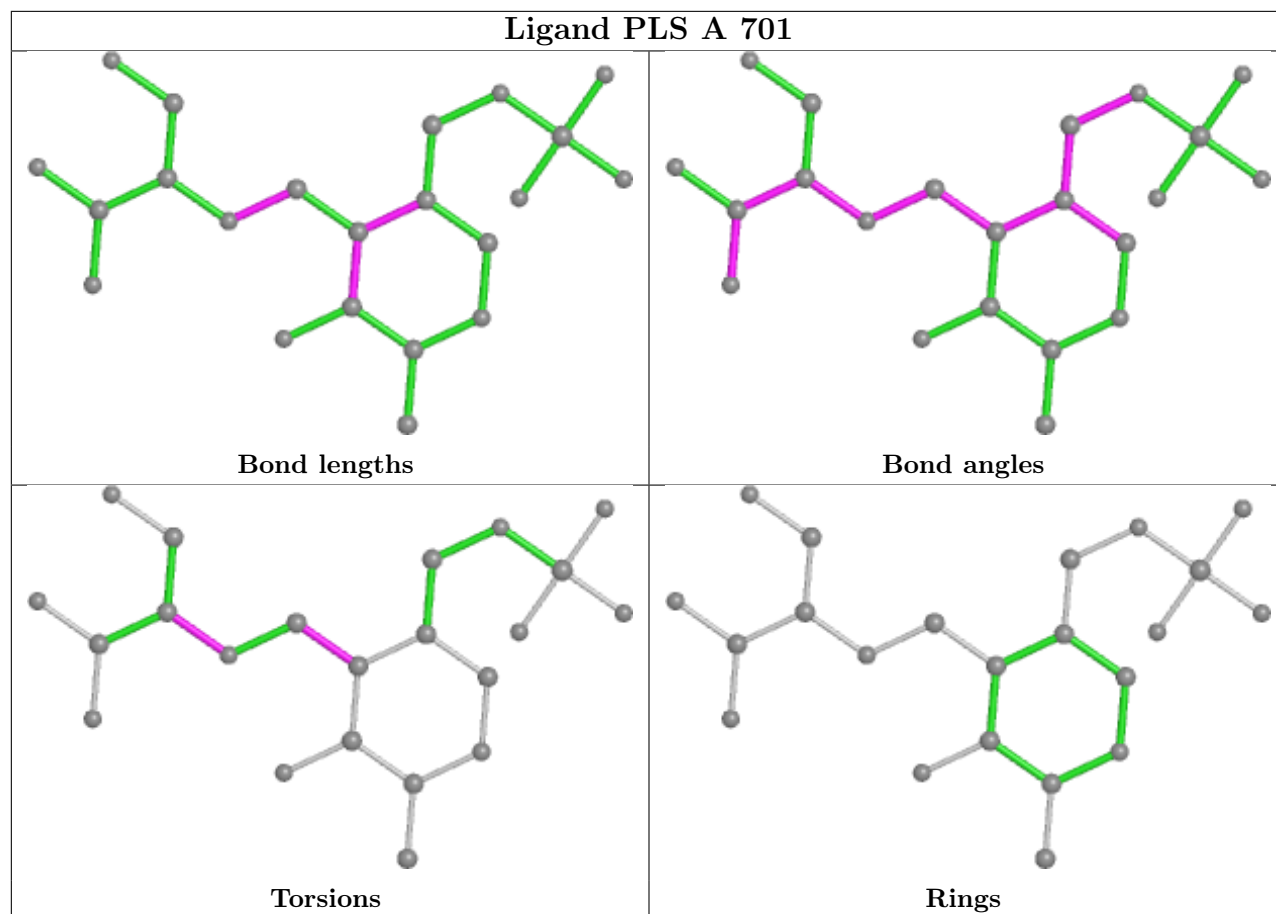
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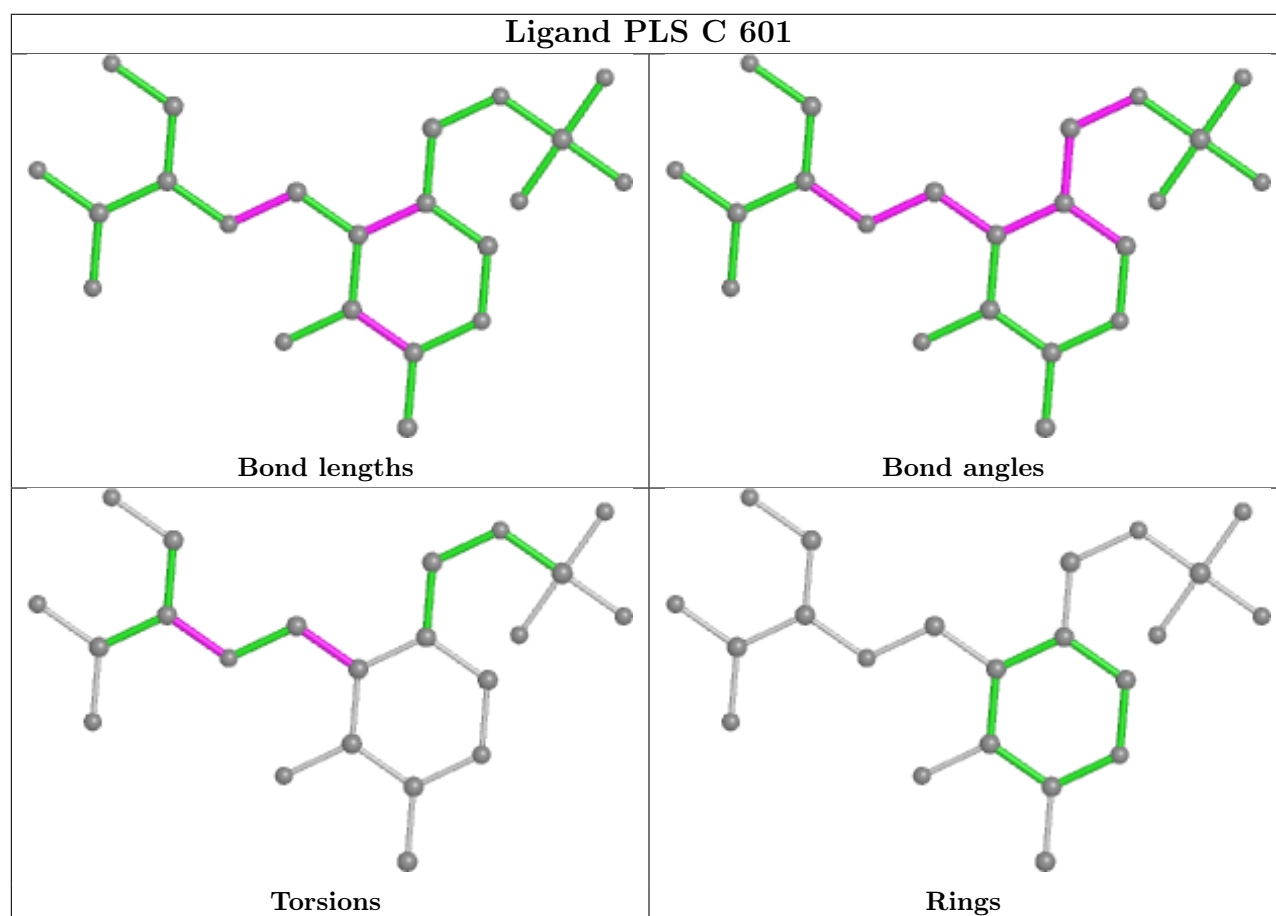
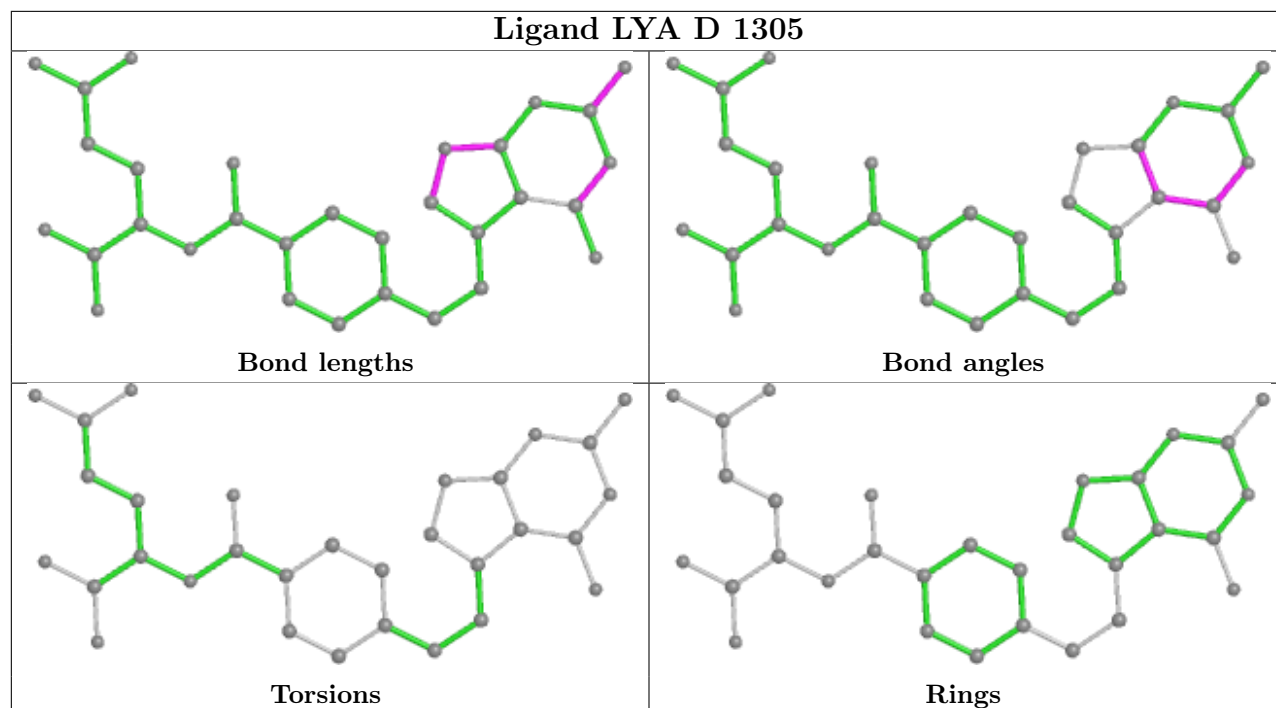
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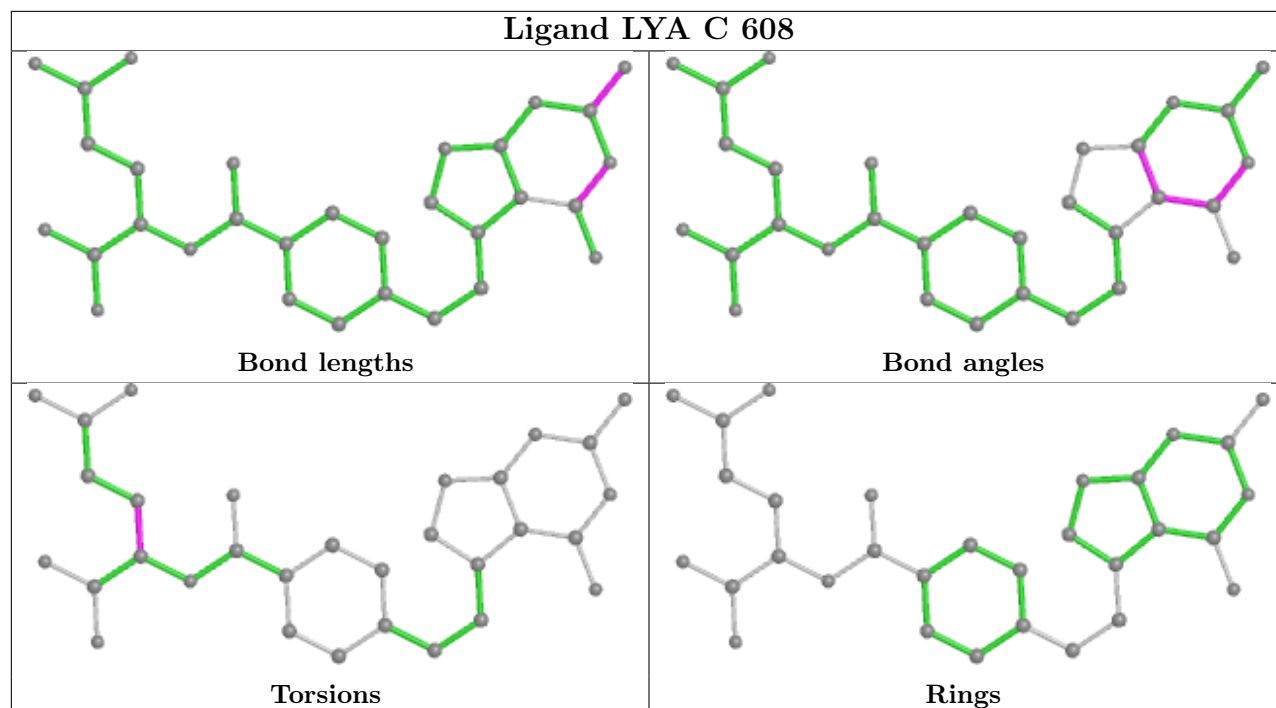
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	614	EDO	4	0
4	A	710	LYA	4	0
4	D	1305	LYA	3	0
3	A	703	EDO	1	0
3	C	605	EDO	1	0
2	C	601	PLS	1	0
4	C	608	LYA	5	0

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	475/480 (98%)	-0.26	16 (3%) 45 51	12, 19, 49, 83	0
1	B	475/480 (98%)	-0.21	20 (4%) 36 41	13, 21, 52, 83	0
1	C	475/480 (98%)	-0.21	9 (1%) 66 72	12, 18, 40, 84	0
1	D	480/480 (100%)	-0.06	24 (5%) 28 32	12, 21, 57, 89	0
All	All	1905/1920 (99%)	-0.18	69 (3%) 42 49	12, 20, 50, 89	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	421	VAL	10.6
1	D	468	GLN	8.7
1	B	43	SER	8.1
1	B	468	GLN	6.8
1	A	43	SER	6.1
1	B	47	TRP	6.1
1	D	470	THR	6.0
1	A	46	SER	5.4
1	C	424	MET	5.3
1	A	468	GLN	5.3
1	A	45	SER	5.2
1	D	423	ALA	5.0
1	C	307	LYS	4.7
1	B	424	MET	4.4
1	D	477	ALA	4.3
1	B	421	VAL	4.2
1	B	310	LYS	4.0
1	C	423	ALA	3.9
1	D	476	VAL	3.9
1	A	470	THR	3.7
1	D	481	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	476	VAL	3.6
1	B	481	SER	3.6
1	D	480	GLN	3.5
1	A	44	ARG	3.5
1	A	112[A]	TYR	3.5
1	B	45	SER	3.4
1	D	424	MET	3.4
1	D	469	GLY	3.3
1	B	480	GLN	3.2
1	A	421	VAL	3.2
1	D	517	GLU	3.2
1	D	465	ALA	3.1
1	D	472	LEU	3.1
1	A	305	ILE	3.0
1	B	477	ALA	3.0
1	D	474	ASP	2.9
1	B	46	SER	2.9
1	D	473	LYS	2.8
1	A	47	TRP	2.8
1	C	517	GLU	2.8
1	B	473	LYS	2.8
1	A	477	ALA	2.7
1	B	467	SER	2.7
1	D	38	SER	2.6
1	A	185	ASP	2.6
1	B	485	LEU	2.6
1	D	112[A]	TYR	2.5
1	B	517	GLU	2.5
1	D	471	LYS	2.4
1	D	479	MET	2.4
1	D	186	THR	2.4
1	D	467	SER	2.4
1	A	481	SER	2.3
1	B	44	ARG	2.3
1	A	424	MET	2.3
1	D	484	LYS	2.3
1	C	46	SER	2.3
1	A	422	SER	2.2
1	C	425	VAL	2.2
1	C	308	GLN	2.2
1	D	425	VAL	2.2
1	B	425	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	483	GLU	2.2
1	A	480	GLN	2.1
1	C	422	SER	2.1
1	B	470	THR	2.1
1	D	485	LEU	2.1
1	C	305	ILE	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
4	LYA	D	1305	31/31	0.60	0.28	74,77,92,92	31
4	LYA	C	608	31/31	0.65	0.24	45,50,69,71	31
3	EDO	D	1303	4/4	0.73	0.16	69,70,70,71	0
3	EDO	B	607	4/4	0.74	0.16	71,73,73,74	0
3	EDO	C	609	4/4	0.76	0.20	54,54,56,57	0
4	LYA	A	710	31/31	0.76	0.20	44,51,69,71	31
3	EDO	C	612	4/4	0.78	0.17	43,47,49,51	0
3	EDO	C	611	4/4	0.81	0.18	52,53,53,55	0
3	EDO	C	605	4/4	0.81	0.14	36,40,43,43	0
3	EDO	B	610	4/4	0.81	0.10	76,76,77,77	0
3	EDO	C	615	4/4	0.82	0.15	42,42,43,43	0
3	EDO	B	602	4/4	0.84	0.16	48,49,51,52	0
3	EDO	C	610	4/4	0.84	0.09	65,65,65,65	0
3	EDO	D	1306	4/4	0.84	0.14	53,54,54,54	0
3	EDO	C	602	4/4	0.85	0.12	31,32,34,35	0
3	EDO	A	708	4/4	0.85	0.15	55,56,57,59	0
3	EDO	B	606	4/4	0.86	0.14	55,56,56,57	0

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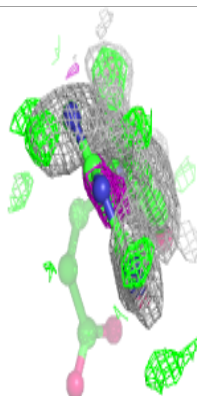
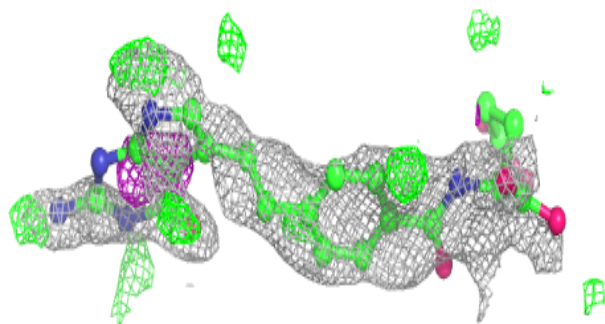
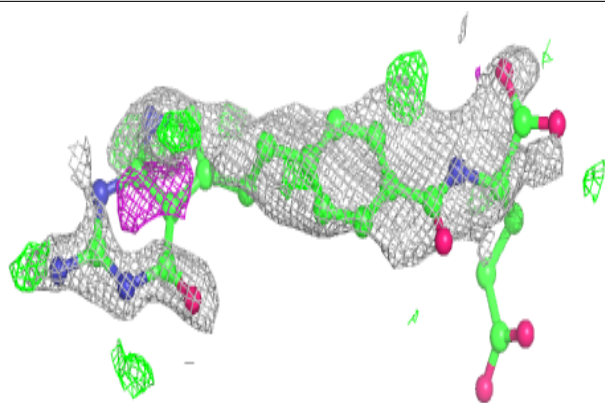
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	711	4/4	0.86	0.10	56,56,57,57	0
3	EDO	B	609	4/4	0.86	0.20	47,47,48,49	0
3	EDO	A	705	4/4	0.86	0.19	49,50,50,52	0
3	EDO	B	605	4/4	0.87	0.11	49,50,50,51	0
3	EDO	C	607	4/4	0.87	0.12	41,44,46,48	0
3	EDO	C	603	4/4	0.88	0.15	48,48,49,52	0
3	EDO	D	1307	4/4	0.89	0.15	37,40,41,44	0
3	EDO	A	707	4/4	0.90	0.13	47,48,49,50	0
3	EDO	A	706	4/4	0.90	0.10	38,41,45,47	0
3	EDO	B	604	4/4	0.91	0.13	41,43,44,46	0
3	EDO	D	1309	4/4	0.92	0.12	47,48,49,50	0
3	EDO	D	1301	4/4	0.92	0.09	29,33,35,40	0
3	EDO	B	608	4/4	0.92	0.15	34,36,37,38	0
3	EDO	D	1308	4/4	0.92	0.09	43,44,45,45	0
3	EDO	B	603	4/4	0.93	0.17	23,26,29,32	0
3	EDO	A	703	4/4	0.93	0.17	38,39,39,40	0
3	EDO	D	1304	4/4	0.94	0.11	33,36,37,37	0
3	EDO	C	614	4/4	0.94	0.11	36,38,39,39	0
3	EDO	D	1302	4/4	0.94	0.11	22,23,28,32	0
3	EDO	A	709	4/4	0.94	0.12	35,37,40,43	0
5	SER	C	613	7/7	0.94	0.14	38,39,41,43	0
3	EDO	A	704	4/4	0.95	0.07	33,36,38,40	0
3	EDO	C	606	4/4	0.95	0.09	27,29,29,30	0
3	EDO	C	604	4/4	0.95	0.12	36,36,38,38	0
3	EDO	A	702	4/4	0.97	0.10	23,25,29,33	0
2	PLS	A	701	22/22	0.98	0.07	13,16,19,32	0
2	PLS	B	601	22/22	0.98	0.07	14,16,25,35	0
2	PLS	C	601	22/22	0.98	0.08	14,16,25,34	0
6	PLP	D	1310	15/16	0.98	0.07	14,17,20,21	0

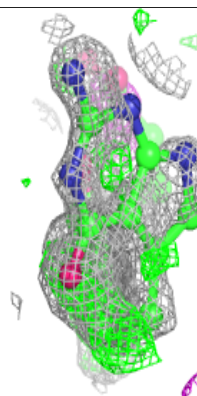
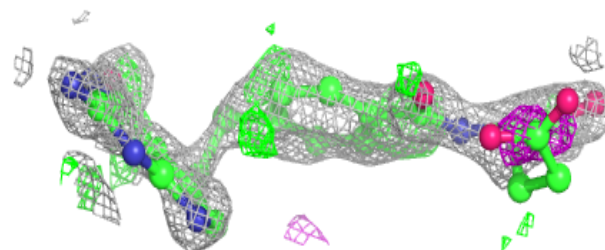
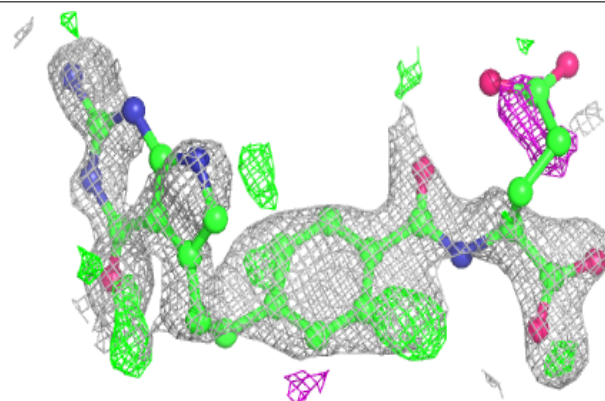
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LYA D 1305:

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

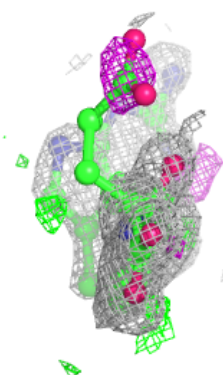
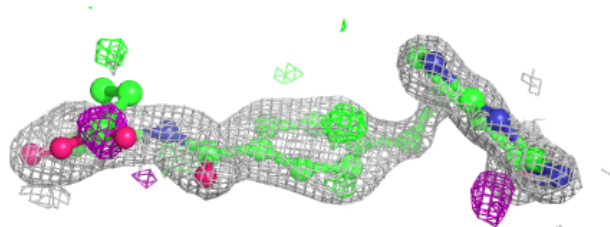
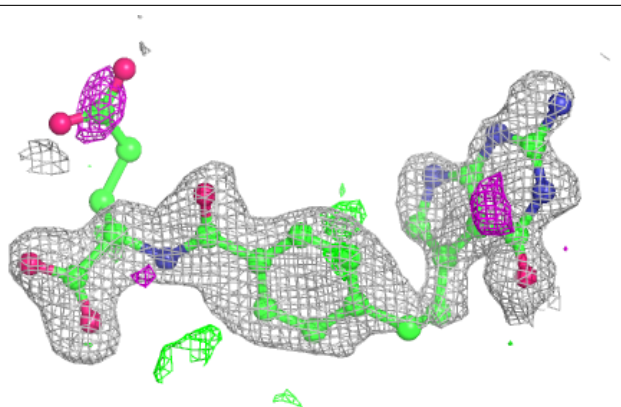
**Electron density around LYA C 608:**

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



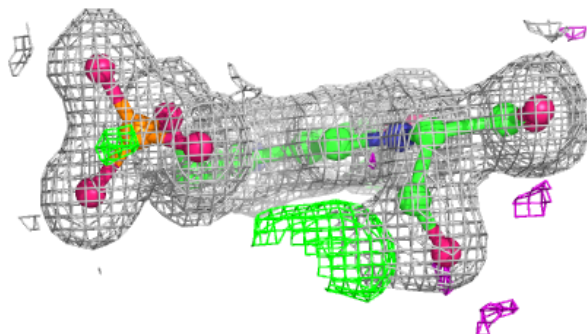
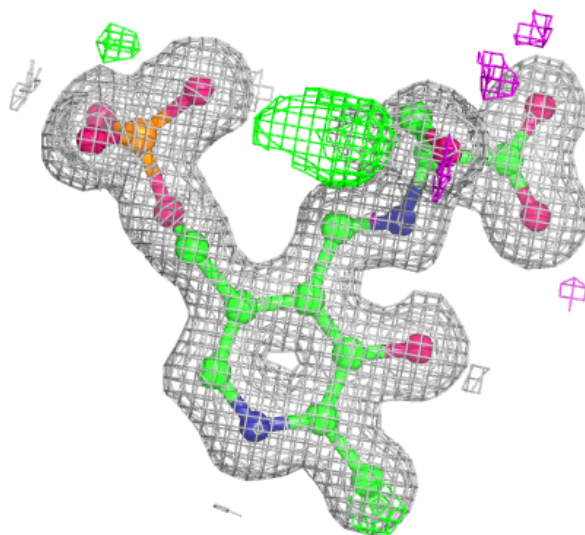
Electron density around LYA A 710:

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



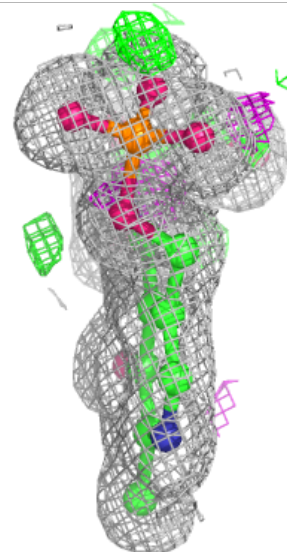
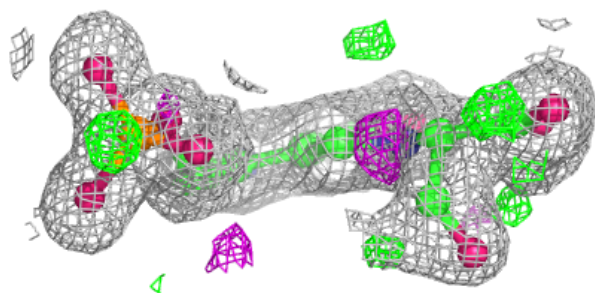
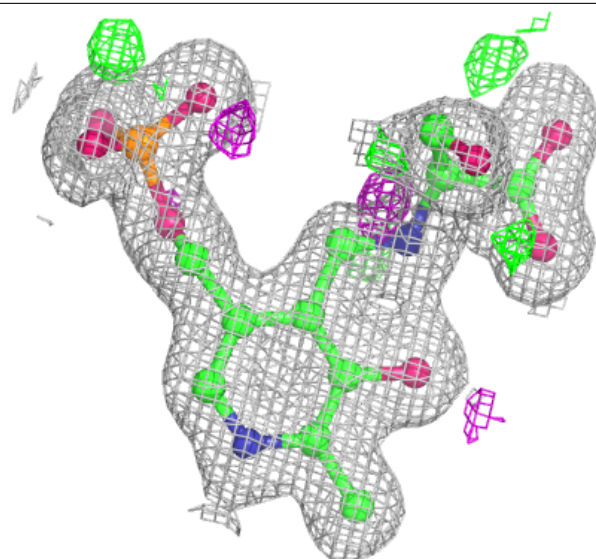
Electron density around PLS A 701:

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



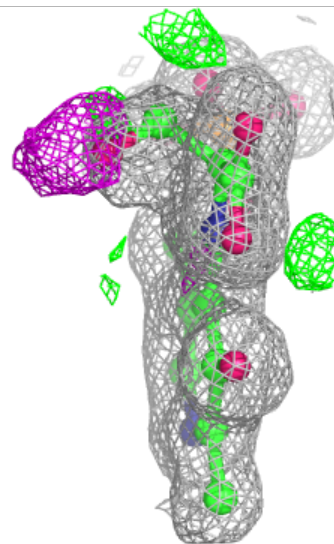
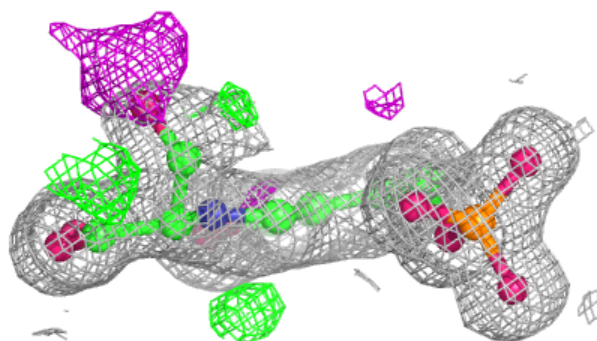
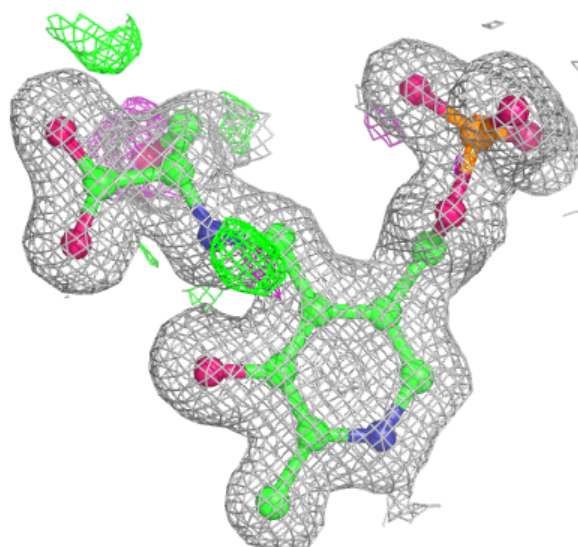
Electron density around PLS B 601:

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



Electron density around PLS C 601:

$2mF_o-DF_c$ (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.