



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:34 PM UTC

PDB ID : 5X30 / pdb_00005x30
Title : Crystal structure of Pseudomonas putida methionine gamma-lyase C116H mutant with L-homocysteine intermediates.
Authors : Shiba, T.; Sato, D.; Harada, S.
Deposited on : 2017-02-02
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

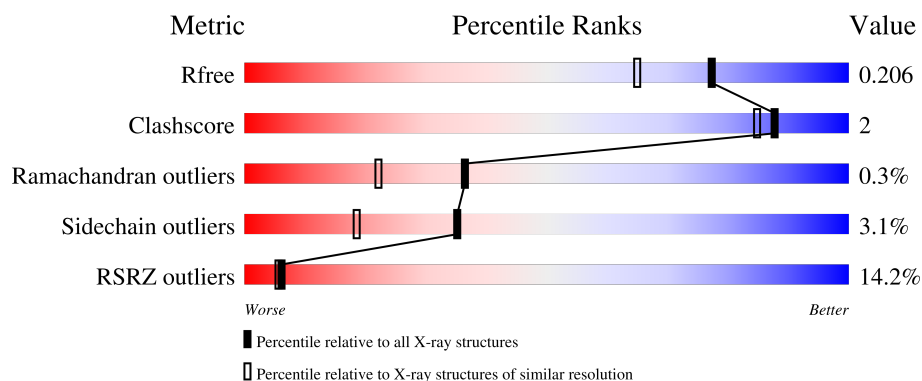
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	398	16% 94% ...
1	C	398	13% 91% 7% ..
2	B	398	11% 90% 8% ..
2	D	398	16% 94% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13001 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 L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	P	S	0	0	0
			2970	1874	525	554	1	16			
1	C	393	Total	C	N	O	P	S	0	0	0
			2975	1877	526	555	1	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	HIS	CYS	engineered mutation	UNP P13254
C	116	HIS	CYS	engineered mutation	UNP P13254

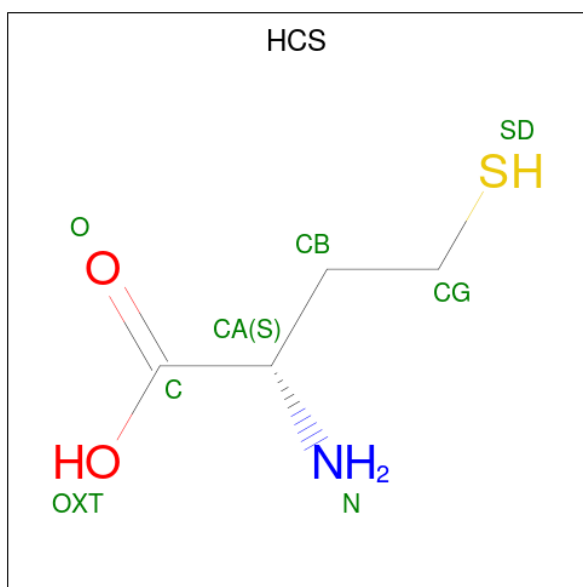
- Molecule 2 is a protein called L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	392	Total	C	N	O	S	0	1	0
			2963	1870	525	552	16			
2	D	398	Total	C	N	O	S	0	1	0
			3010	1898	537	558	17			

There are 2 discrepancies between the modelled and reference sequences:

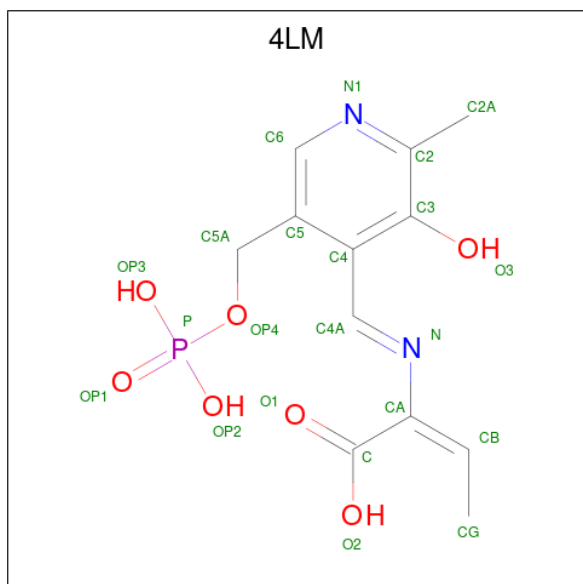
Chain	Residue	Modelled	Actual	Comment	Reference
B	116	HIS	CYS	engineered mutation	UNP P13254
D	116	HIS	CYS	engineered mutation	UNP P13254

- Molecule 3 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (CCD ID: HCS) (formula: C₄H₉NO₂S).



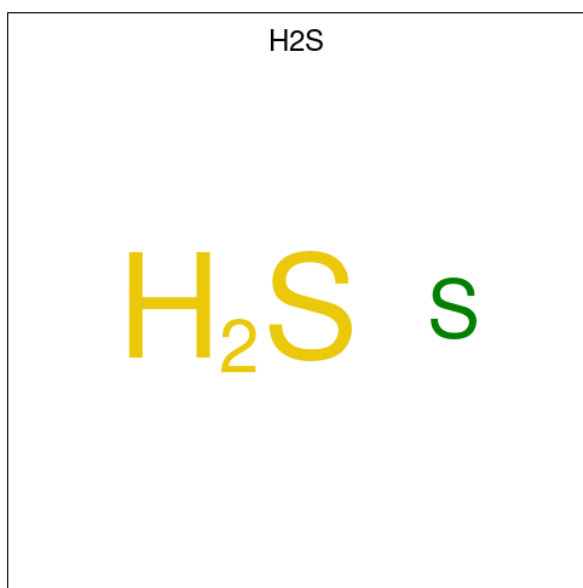
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			8	4	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			8	4	1	2	1		

- Molecule 4 is (2E)-2-[[[(1E)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino]but-2-enoic acid (CCD ID: 4LM) (formula: C₁₂H₁₅N₂O₇P).



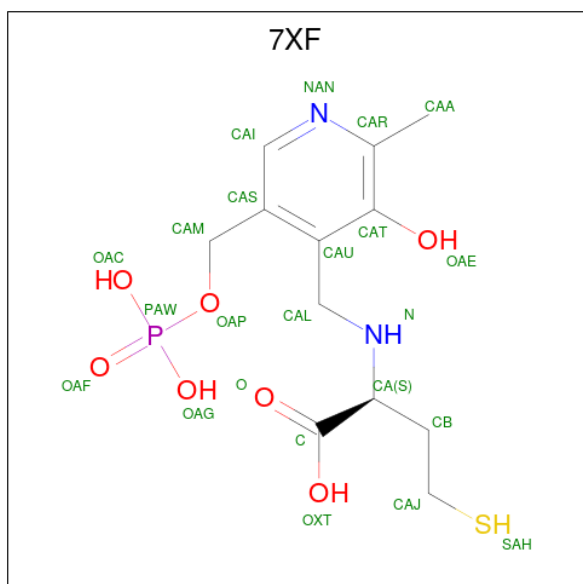
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

- Molecule 5 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	S	0	0
			1	1		

- Molecule 6 is (2 {S})-2-[[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methyloamino]-4-sulfanyl-butanoic acid (CCD ID: 7XF) (formula: C₁₂H₁₉N₂O₇PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	S	0	0
			23	12	2	7	1	1		

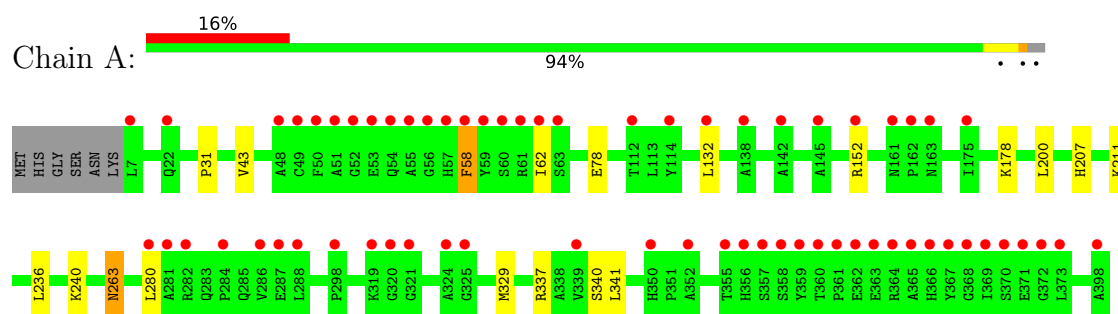
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	194	Total 194	O 194	0	0
7	B	292	Total 292	O 292	0	0
7	C	268	Total 268	O 268	0	0
7	D	267	Total 267	O 267	0	0

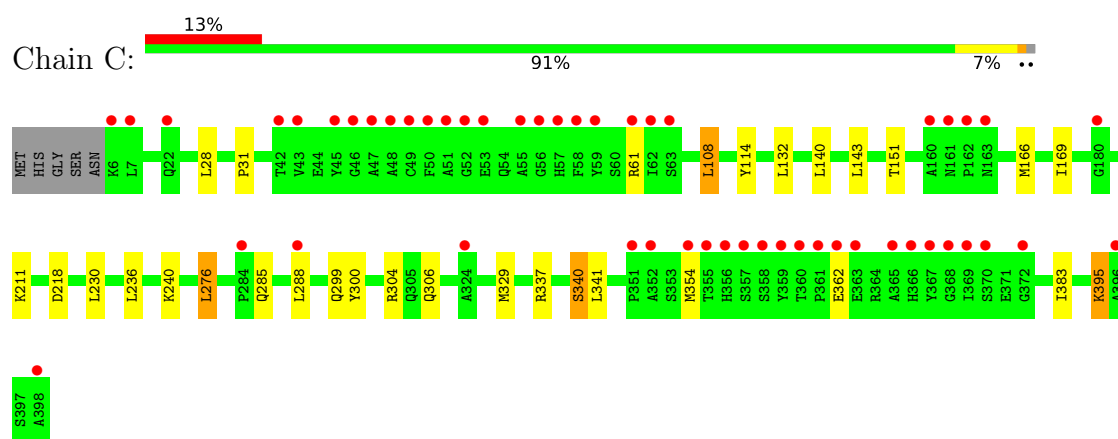
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

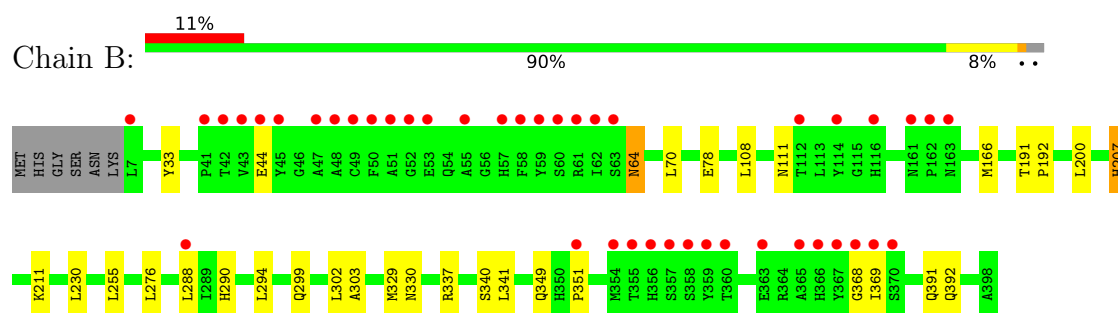
- Molecule 1: L-methionine gamma-lyase



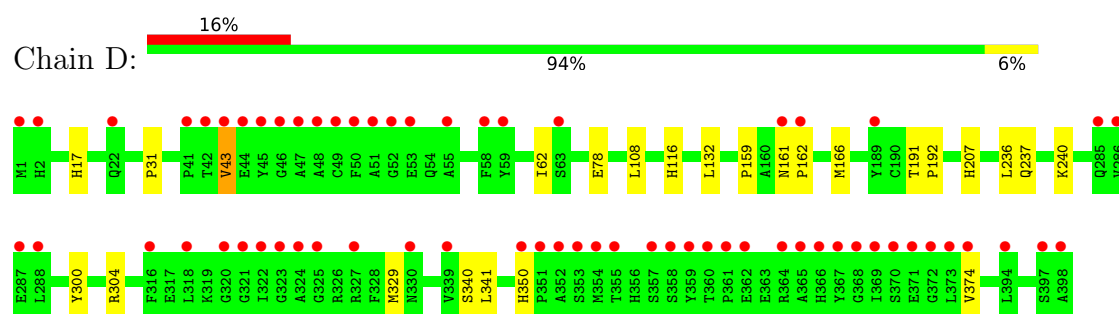
- Molecule 1: L-methionine gamma-lyase



- Molecule 2: L-methionine gamma-lyase



- Molecule 2: L-methionine gamma-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.75Å 152.97Å 80.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-1.70) 99.4 (20.00-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.170 , 0.195 0.180 , 0.206	Depositor DCC
R_{free} test set	10413 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13001	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7XF, H2S, HCS, LLP, 4LM

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	0.63	0/3010	0.83	0/4086
1	C	0.67	1/3015 (0.0%)	0.83	0/4093
2	B	0.68	1/3028 (0.0%)	0.83	0/4111
2	D	0.68	0/3077	0.82	0/4175
All	All	0.66	2/12130 (0.0%)	0.83	0/16465

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	218	ASP	C-N	-7.71	1.23	1.33
2	B	64	ASN	CA-C	5.04	1.58	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	207	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2970	0	2927	7	0
1	C	2975	0	2929	14	0
2	B	2963	0	2926	17	0
2	D	3010	0	2975	15	0
3	A	8	0	8	0	0
3	C	8	0	8	2	0
4	B	22	0	11	2	0
5	B	1	0	0	0	0
6	D	23	0	0	0	0
7	A	194	0	0	0	0
7	B	292	0	0	1	0
7	C	268	0	0	1	0
7	D	267	0	0	3	0
All	All	13001	0	11784	48	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 (48) 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:C:169:ILE:H	1:C:306:GLN:HE22	1.37	0.73
1:C:61:ARG:HH22	2:D:116:HIS:CD2	2.10	0.69
2:B:288:LEU:HD21	2:B:290:HIS:NE2	2.08	0.68
2:B:211:LYS:HZ1	4:B:401:4LM:C4A	2.06	0.67
2:B:166:MET:H	2:B:299:GLN:HE22	1.43	0.65
1:A:43:VAL:H	2:B:330:ASN:HD21	1.46	0.64
2:D:329:MET:HE2	2:D:350:HIS:HB2	1.80	0.62
2:B:211:LYS:NZ	4:B:401:4LM:C4A	2.65	0.60
1:C:166:MET:H	1:C:299:GLN:HE22	1.51	0.59
1:C:329:MET:HE3	1:C:337:ARG:HG2	1.88	0.54
1:C:236:LEU:O	1:C:240:LYS:HE3	2.08	0.54
2:B:33:TYR:CE2	1:C:31:PRO:HG3	2.45	0.52
2:D:159:PRO:HG3	2:D:166:MET:HE2	1.90	0.51
2:B:166:MET:HE1	2:B:303:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:300:TYR:CZ	2:D:304:ARG:HD2	2.45	0.51
1:C:276:LEU:HD13	1:C:383:ILE:HD11	1.93	0.50
1:C:354:MET:HG3	2:D:43:VAL:HG22	1.93	0.49
2:B:288:LEU:CD2	2:B:290:HIS:CE1	2.95	0.48
2:D:78:GLU:OE1	2:D:207:HIS:HE1	1.97	0.48
2:B:368:GLY:C	2:B:369:ILE:HD12	2.39	0.47
2:B:78:GLU:OE2	2:B:207:HIS:HE1	1.98	0.47
2:B:329:MET:HE3	2:B:337:ARG:HG2	1.97	0.46
1:A:78:GLU:OE2	1:A:207:HIS:CE1	2.69	0.46
2:B:78:GLU:OE2	2:B:207:HIS:CE1	2.69	0.45
2:D:236:LEU:O	2:D:240:LYS:HE3	2.15	0.45
1:C:114:TYR:CE1	3:C:501:HCS:HG2	2.51	0.45
2:D:78:GLU:OE1	2:D:207:HIS:CE1	2.69	0.45
2:D:237:GLN:NE2	7:D:602:HOH:O	2.47	0.45
2:D:17:HIS:HD2	7:D:845:HOH:O	1.99	0.45
1:A:329:MET:HE3	1:A:337:ARG:HG2	1.97	0.45
1:A:31:PRO:HB2	2:D:31:PRO:HB2	1.99	0.45
2:B:288:LEU:C	2:B:288:LEU:HD23	2.42	0.44
2:D:191:THR:HB	2:D:192:PRO:HD2	1.98	0.44
1:A:58:PHE:CZ	1:A:62:ILE:HG21	2.53	0.44
2:B:288:LEU:HD21	2:B:290:HIS:CE1	2.53	0.44
2:D:329:MET:HE2	2:D:350:HIS:CB	2.48	0.44
1:A:263:ASN:HD22	1:A:263:ASN:H	1.66	0.43
2:B:191:THR:HB	2:B:192:PRO:HD2	2.01	0.43
1:A:236:LEU:O	1:A:240:LYS:HE3	2.18	0.43
1:C:108:LEU:HD22	1:C:151:THR:HG21	2.01	0.42
1:C:340:SER:HA	3:C:501:HCS:CB	2.49	0.42
2:B:70:LEU:HD21	2:B:255:LEU:HD23	2.01	0.42
1:C:300:TYR:CZ	1:C:304:ARG:HD2	2.54	0.42
2:B:349:GLN:NE2	7:B:505:HOH:O	2.51	0.42
2:D:62:ILE:HA	7:D:651:HOH:O	2.19	0.42
1:C:230:LEU:HD12	7:C:617:HOH:O	2.20	0.41
1:C:395:LYS:N	1:C:395:LYS:HD3	2.34	0.41
2:D:161:ASN:HA	2:D:162:PRO:HA	1.92	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	389/398 (98%)	376 (97%)	12 (3%)	1 (0%)	36	22
1	C	390/398 (98%)	380 (97%)	9 (2%)	1 (0%)	36	22
2	B	391/398 (98%)	380 (97%)	10 (3%)	1 (0%)	36	22
2	D	397/398 (100%)	386 (97%)	10 (2%)	1 (0%)	36	22
All	All	1567/1592 (98%)	1522 (97%)	41 (3%)	4 (0%)	36	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	340	SER
1	C	340	SER
2	D	340	SER
1	A	340	SER

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	301/306 (98%)	293 (97%)	8 (3%)	39	23
1	C	301/306 (98%)	290 (96%)	11 (4%)	30	14
2	B	303/307 (99%)	290 (96%)	13 (4%)	26	10
2	D	308/307 (100%)	303 (98%)	5 (2%)	55	41
All	All	1213/1226 (99%)	1176 (97%)	37 (3%)	35	18

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	132	LEU
1	A	152	ARG
1	A	178	LYS
1	A	200	LEU
1	A	263	ASN
1	A	280	LEU
1	A	341	LEU
2	B	44	GLU
2	B	64	ASN
2	B	108	LEU
2	B	111	ASN
2	B	200	LEU
2	B	230	LEU
2	B	276	LEU
2	B	294	LEU
2	B	302	LEU
2	B	341	LEU
2	B	351	PRO
2	B	391	GLN
2	B	392	GLN
1	C	28	LEU
1	C	108	LEU
1	C	132	LEU
1	C	140	LEU
1	C	143	LEU
1	C	276	LEU
1	C	285	GLN
1	C	288	LEU
1	C	341	LEU
1	C	362	GLU
1	C	395	LYS
2	D	43	VAL
2	D	108	LEU
2	D	132	LEU
2	D	341	LEU
2	D	374	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	22	GLN
1	A	24	HIS
1	A	68	ASN
1	A	163	ASN
1	A	207	HIS
1	A	263	ASN
1	A	274	GLN
1	A	305	GLN
2	B	57	HIS
2	B	64	ASN
2	B	68	ASN
2	B	111	ASN
2	B	207	HIS
2	B	237	GLN
2	B	299	GLN
2	B	330	ASN
2	B	349	GLN
2	B	392	GLN
1	C	34	GLN
1	C	57	HIS
1	C	68	ASN
1	C	165	HIS
1	C	187	ASN
1	C	290	HIS
1	C	299	GLN
1	C	305	GLN
1	C	306	GLN
2	D	17	HIS
2	D	24	HIS
2	D	34	GLN
2	D	68	ASN
2	D	116	HIS
2	D	207	HIS
2	D	274	GLN
2	D	330	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	C	211	1	23,24,25	2.69	5 (21%)	25,32,34	1.40	7 (28%)
1	LLP	A	211	1	23,24,25	2.69	5 (21%)	25,32,34	1.42	5 (20%)

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	C	211	1	-	5/16/17/19	0/1/1/1
1	LLP	A	211	1	-	5/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	LLP	C3-C2	7.30	1.48	1.41
1	A	211	LLP	C3-C2	6.70	1.47	1.41
1	A	211	LLP	C4-C5	6.11	1.50	1.42
1	C	211	LLP	C4'-NZ	6.03	1.47	1.27
1	A	211	LLP	C4'-NZ	5.95	1.47	1.27
1	C	211	LLP	C4-C3	5.46	1.50	1.41
1	A	211	LLP	C4-C3	5.16	1.49	1.41
1	C	211	LLP	C4-C5	5.04	1.49	1.42
1	C	211	LLP	C4-C4'	3.13	1.53	1.46
1	A	211	LLP	C4-C4'	2.77	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LLP	C6-N1-C2	3.15	124.91	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LLP	C2'-C2-N1	2.79	122.90	117.64
1	C	211	LLP	C6-N1-C2	2.68	124.05	119.20
1	A	211	LLP	C4-C3-C2	-2.38	118.80	120.14
1	A	211	LLP	OP3-P-OP2	2.38	116.73	107.80
1	C	211	LLP	C3-C4-C5	-2.35	116.39	118.28
1	C	211	LLP	C3-C2-N1	-2.22	118.16	120.96
1	C	211	LLP	OP4-P-OP1	-2.22	100.43	106.44
1	C	211	LLP	C4-C4'-NZ	-2.21	113.84	124.04
1	C	211	LLP	OP2-P-OP1	2.10	119.02	110.83
1	C	211	LLP	C2'-C2-N1	2.04	121.49	117.64
1	A	211	LLP	C3-C2-N1	-2.01	118.43	120.96

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	C	211	LLP	O-C-CA-CB
1	C	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	CG-CD-CE-NZ
1	C	211	LLP	CA-CB-CG-CD
1	C	211	LLP	CD-CE-NZ-C4'
1	C	211	LLP	C3-C4-C4'-NZ
1	A	211	LLP	C3-C4-C4'-NZ
1	A	211	LLP	CD-CE-NZ-C4'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is modelled with single atom - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	4LM	B	401	-	21,22,22	1.74	5 (23%)	26,31,31	1.92	7 (26%)
3	HCS	C	501	-	6,7,7	1.18	1 (16%)	5,8,8	3.02	3 (60%)
3	HCS	A	501	-	6,7,7	1.02	1 (16%)	5,8,8	4.00	2 (40%)
6	7XF	D	501	-	23,23,23	2.22	4 (17%)	27,32,32	2.55	5 (18%)

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
4	4LM	B	401	-	-	0/15/17/17	0/1/1/1
3	HCS	C	501	-	-	1/7/7/7	-
3	HCS	A	501	-	-	2/7/7/7	-
6	7XF	D	501	-	-	5/18/18/18	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	501	7XF	CB-CA	-7.35	1.36	1.53
6	D	501	7XF	CAR-NAN	3.84	1.40	1.33
4	B	401	4LM	C2-N1	3.53	1.40	1.33
4	B	401	4LM	C4-C4A	3.35	1.53	1.46
4	B	401	4LM	P-OP2	-2.70	1.44	1.54
6	D	501	7XF	CA-C	-2.56	1.46	1.52
3	C	501	HCS	OXT-C	-2.48	1.22	1.30
6	D	501	7XF	CAT-CAR	-2.47	1.38	1.41
3	A	501	HCS	OXT-C	-2.34	1.23	1.30
4	B	401	4LM	C3-C2	-2.25	1.38	1.41
4	B	401	4LM	C2A-C2	2.00	1.53	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	501	7XF	CB-CAJ-SAH	-9.96	103.36	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCS	CB-CG-SD	-8.23	105.16	113.74
4	B	401	4LM	O2-C-CA	5.86	122.80	113.40
3	C	501	HCS	CG-CB-CA	5.54	122.19	113.14
6	D	501	7XF	CAL-N-CA	5.12	123.45	113.84
4	B	401	4LM	O2-C-O1	-3.46	115.67	123.90
4	B	401	4LM	C3-C2-N1	-3.25	116.87	120.96
4	B	401	4LM	C4-C3-C2	3.24	121.97	120.14
6	D	501	7XF	OXT-C-O	-3.23	116.74	124.08
3	C	501	HCS	CB-CA-N	3.21	118.48	110.12
6	D	501	7XF	CAT-CAR-NAN	-2.86	117.35	120.96
3	A	501	HCS	OXT-C-O	-2.63	118.12	124.08
4	B	401	4LM	OP2-P-OP4	2.44	113.02	106.67
4	B	401	4LM	C2A-C2-N1	2.42	122.20	117.64
6	D	501	7XF	OXT-C-CA	2.38	121.55	113.51
4	B	401	4LM	OP4-C5A-C5	-2.16	105.31	109.36
3	C	501	HCS	OXT-C-O	-2.12	119.28	124.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HCS	N-CA-CB-CG
3	A	501	HCS	C-CA-CB-CG
6	D	501	7XF	N-CAL-CAU-CAS
3	C	501	HCS	CA-CB-CG-SD
6	D	501	7XF	N-CAL-CAU-CAT
6	D	501	7XF	CB-CA-N-CAL
6	D	501	7XF	C-CA-N-CAL
6	D	501	7XF	N-CA-CB-CAJ

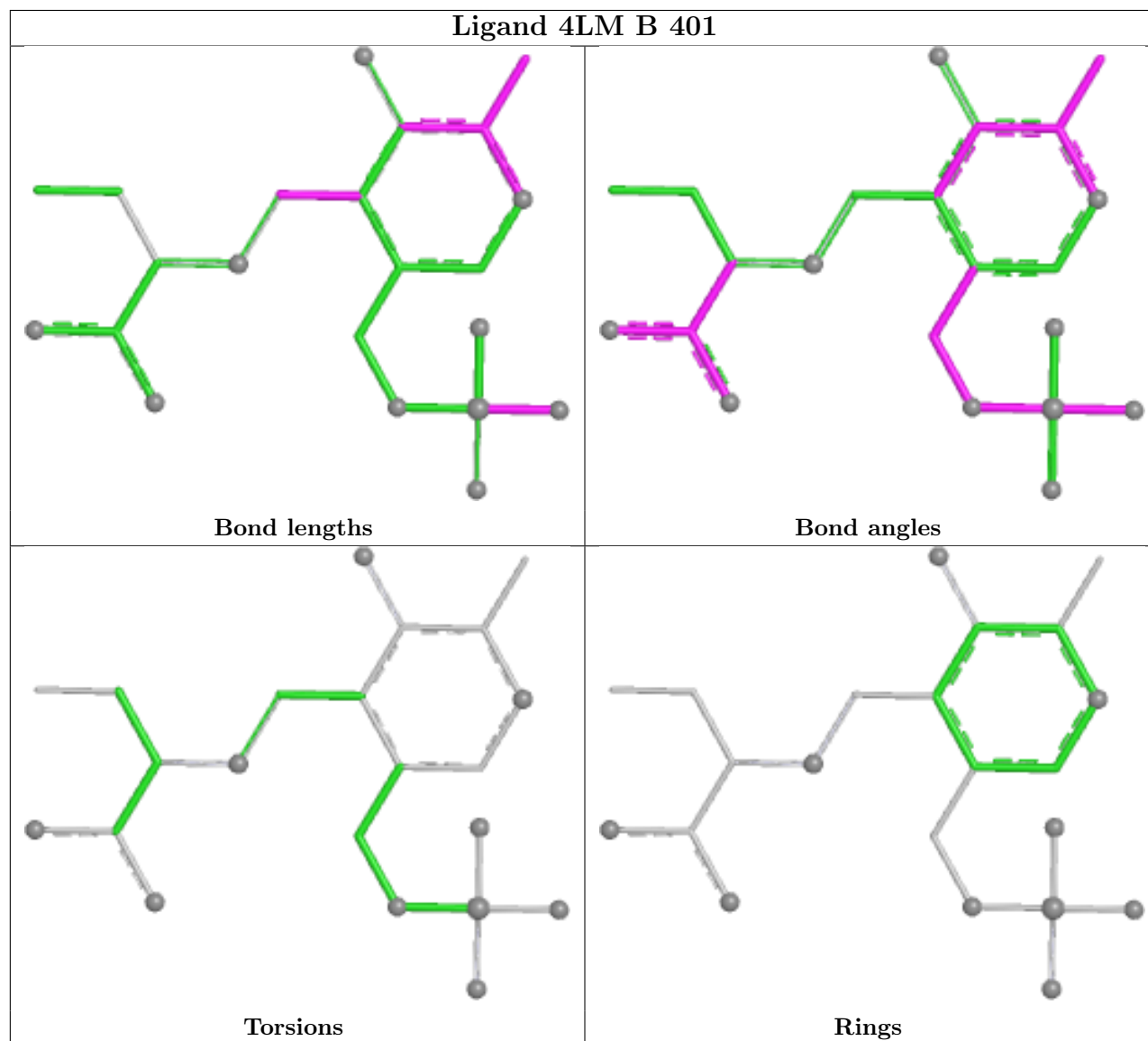
There are no ring outliers.

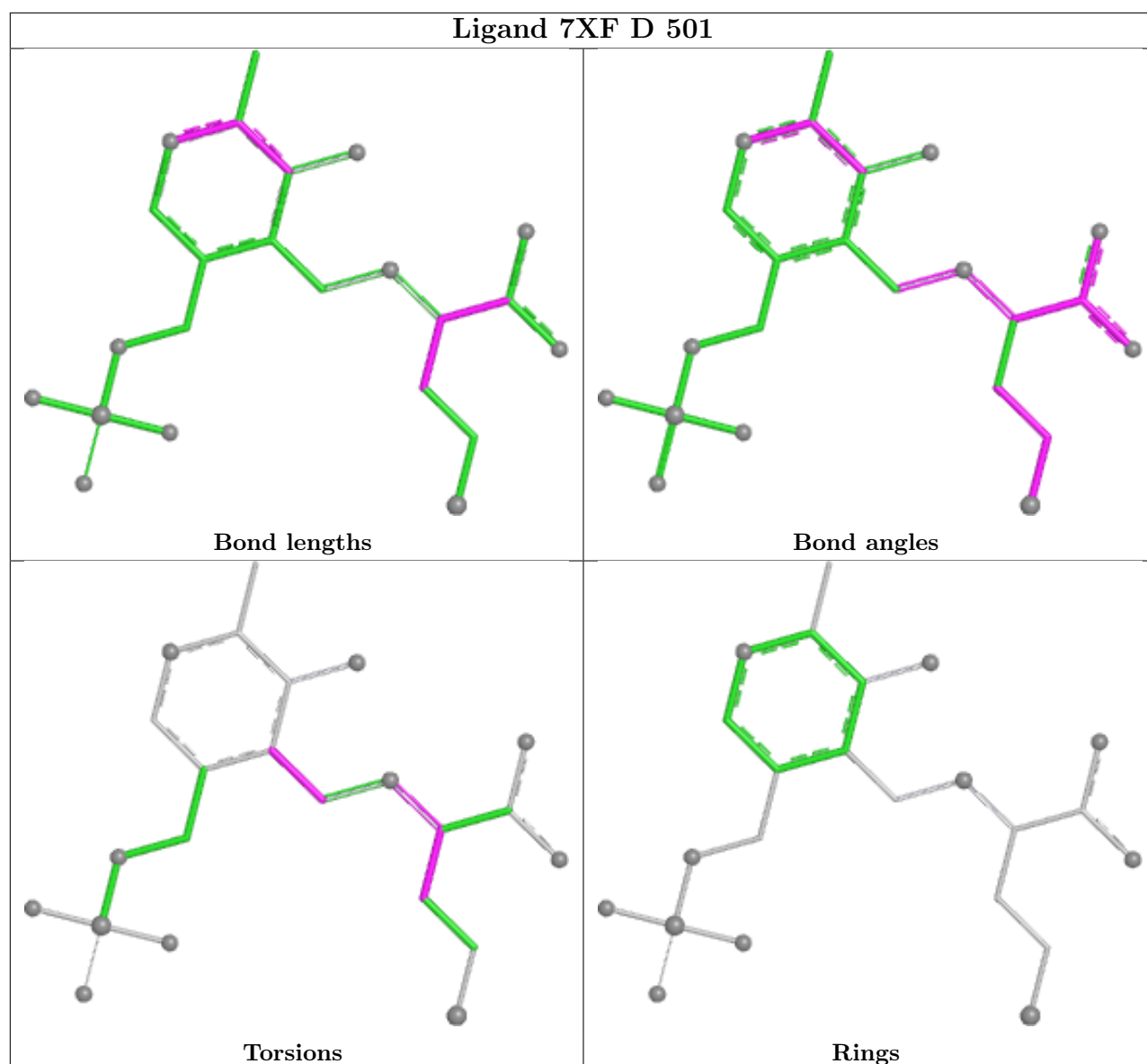
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	4LM	2	0
3	C	501	HCS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	391/398 (98%)	0.77	65 (16%)	4 4	15, 29, 71, 119	0
1	C	392/398 (98%)	0.35	51 (13%)	7 7	13, 23, 68, 98	0
2	B	392/398 (98%)	0.26	43 (10%)	10 10	8, 21, 57, 112	1 (0%)
2	D	398/398 (100%)	0.45	64 (16%)	4 4	11, 21, 74, 111	1 (0%)
All	All	1573/1592 (98%)	0.46	223 (14%)	6 5	8, 23, 68, 119	2 (0%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	367	TYR	9.6
2	D	51	ALA	8.2
1	A	59	TYR	7.0
1	A	55	ALA	6.9
1	A	365	ALA	6.9
2	B	367	TYR	6.2
1	A	368	GLY	6.0
2	D	367	TYR	6.0
1	A	58	PHE	5.9
2	B	55	ALA	5.9
2	D	365	ALA	5.5
2	D	324	ALA	5.5
2	D	1	MET	5.4
1	A	367	TYR	5.4
2	D	320	GLY	5.2
1	A	359	TYR	5.2
1	A	62	ILE	5.2
2	D	50	PHE	5.1
1	A	361	PRO	5.1
2	B	365	ALA	5.0
2	B	369	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	51	ALA	4.9
1	A	366	HIS	4.9
1	A	369	ILE	4.9
2	B	359	TYR	4.8
1	C	162	PRO	4.7
1	A	357	SER	4.7
2	D	366	HIS	4.7
2	D	55	ALA	4.7
1	A	288	LEU	4.6
1	A	360	THR	4.6
1	A	61	ARG	4.6
2	D	52	GLY	4.6
1	C	62	ILE	4.6
2	D	59	TYR	4.5
2	D	352	ALA	4.5
2	D	372	GLY	4.4
1	C	361	PRO	4.4
2	B	58	PHE	4.4
2	D	2	HIS	4.4
1	A	63	SER	4.3
1	C	55	ALA	4.3
2	B	45	TYR	4.3
1	A	48	ALA	4.2
2	D	47	ALA	4.2
2	D	43	VAL	4.1
2	D	322	ILE	4.1
2	D	323	GLY	4.1
2	B	48	ALA	4.1
1	A	358	SER	4.1
2	D	321	GLY	4.0
1	C	365	ALA	4.0
2	D	398	ALA	4.0
1	C	161	ASN	3.9
1	C	360	THR	3.9
2	D	373	LEU	3.9
2	D	49	CYS	3.9
2	D	350	HIS	3.9
1	A	363	GLU	3.9
1	A	54	GLN	3.9
1	C	59	TYR	3.9
1	C	50	PHE	3.9
1	C	369	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	288	LEU	3.8
2	D	360	THR	3.8
1	A	57	HIS	3.8
1	A	370	SER	3.8
2	D	42	THR	3.8
2	D	355	THR	3.8
1	A	364	ARG	3.7
2	D	161	ASN	3.7
2	B	162	PRO	3.7
2	D	369	ILE	3.7
1	C	6	LYS	3.7
2	B	59	TYR	3.7
1	A	52	GLY	3.7
2	D	325	GLY	3.7
2	D	58	PHE	3.7
2	B	62	ILE	3.6
1	C	45	TYR	3.6
1	C	57	HIS	3.6
1	A	362	GLU	3.5
2	B	52	GLY	3.5
1	C	48	ALA	3.5
2	B	368	GLY	3.5
2	B	7	LEU	3.5
2	D	361	PRO	3.5
2	B	63	SER	3.4
2	B	47	ALA	3.4
2	D	368	GLY	3.4
2	B	114	TYR	3.4
2	B	161	ASN	3.3
1	C	63	SER	3.3
1	C	51	ALA	3.3
2	B	57	HIS	3.3
2	D	359	TYR	3.3
1	A	50	PHE	3.3
1	C	368	GLY	3.2
1	C	398	ALA	3.2
1	C	355	THR	3.2
1	A	162	PRO	3.2
1	A	53	GLU	3.2
2	D	354	MET	3.2
1	A	7	LEU	3.2
2	D	353	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	352	ALA	3.2
2	D	46	GLY	3.1
1	C	47	ALA	3.1
2	D	357	SER	3.1
1	A	350	HIS	3.1
1	A	356	HIS	3.1
1	A	398	ALA	3.1
1	C	58	PHE	3.1
1	C	356	HIS	3.0
1	C	359	TYR	3.0
2	B	41	PRO	3.0
2	B	360	THR	3.0
1	C	358	SER	3.0
1	C	366	HIS	2.9
2	B	60	SER	2.9
1	A	49	CYS	2.9
2	B	49	CYS	2.9
2	B	351	PRO	2.9
1	C	396	ALA	2.8
2	B	358	SER	2.8
2	B	366	HIS	2.8
2	B	355	THR	2.8
2	B	50	PHE	2.8
2	D	48	ALA	2.8
2	B	356	HIS	2.8
2	D	362	GLU	2.8
2	D	286	VAL	2.8
1	A	321	GLY	2.8
2	D	330	ASN	2.7
1	A	60	SER	2.7
1	C	357	SER	2.7
2	D	370	SER	2.7
1	C	362	GLU	2.7
2	D	371	GLU	2.7
1	A	163	ASN	2.7
2	D	339	VAL	2.7
1	A	373	LEU	2.7
1	C	49	CYS	2.7
2	D	63	SER	2.7
1	C	163	ASN	2.7
1	A	352	ALA	2.7
1	C	7	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	288	LEU	2.7
2	D	45	TYR	2.7
2	B	53	GLU	2.6
1	C	370	SER	2.6
2	D	397	SER	2.6
1	A	161	ASN	2.6
1	A	114	TYR	2.6
2	B	43	VAL	2.6
1	C	56	GLY	2.6
2	B	61	ARG	2.6
2	D	44	GLU	2.6
2	D	162	PRO	2.5
1	A	320	GLY	2.5
2	D	316	PHE	2.5
1	C	42	THR	2.5
1	A	142	ALA	2.5
2	B	354	MET	2.5
2	B	363	GLU	2.5
2	B	163	ASN	2.4
1	C	22	GLN	2.4
1	A	175	ILE	2.4
2	B	42	THR	2.4
2	D	364	ARG	2.4
1	A	371	GLU	2.4
1	A	56	GLY	2.4
2	D	285	GLN	2.4
1	A	355	THR	2.4
1	A	286	VAL	2.4
1	C	46	GLY	2.3
1	C	284	PRO	2.3
1	C	351	PRO	2.3
1	A	51	ALA	2.3
1	A	145	ALA	2.3
1	A	152	ARG	2.3
2	D	318	LEU	2.3
2	B	116	HIS	2.3
1	A	339	VAL	2.3
1	C	43	VAL	2.3
2	D	374	VAL	2.3
1	A	287	GLU	2.3
1	A	298	PRO	2.3
1	A	281	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	53	GLU	2.3
1	A	22	GLN	2.3
1	C	53	GLU	2.3
2	D	358	SER	2.3
1	A	284	PRO	2.2
1	A	324	ALA	2.2
1	C	354	MET	2.2
1	C	372	GLY	2.2
2	D	22	GLN	2.2
1	A	282	ARG	2.2
2	B	370	SER	2.2
2	D	287	GLU	2.2
1	A	112	THR	2.2
2	D	41	PRO	2.2
1	A	372	GLY	2.2
2	B	112	THR	2.2
2	B	357	SER	2.2
1	A	138	ALA	2.1
1	C	52	GLY	2.1
1	A	280	LEU	2.1
2	D	351	PRO	2.1
2	D	189	TYR	2.1
1	C	160	ALA	2.1
1	C	180	GLY	2.1
1	A	132	LEU	2.1
2	D	327	ARG	2.1
2	D	394	LEU	2.1
1	A	325	GLY	2.0
1	C	363	GLU	2.0
1	C	61	ARG	2.0
2	B	288	LEU	2.0
2	B	44	GLU	2.0
1	C	324	ALA	2.0
1	A	319	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	A	211	24/25	0.95	0.10	17,26,31,34	0
1	LLP	C	211	24/25	0.97	0.08	14,21,26,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

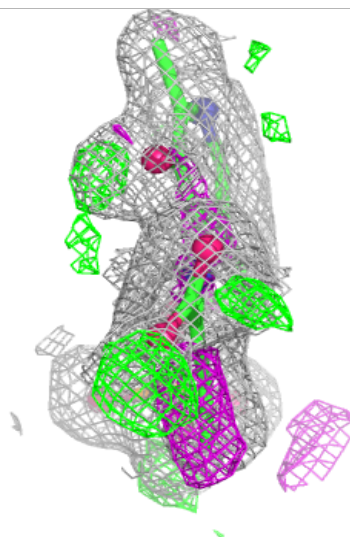
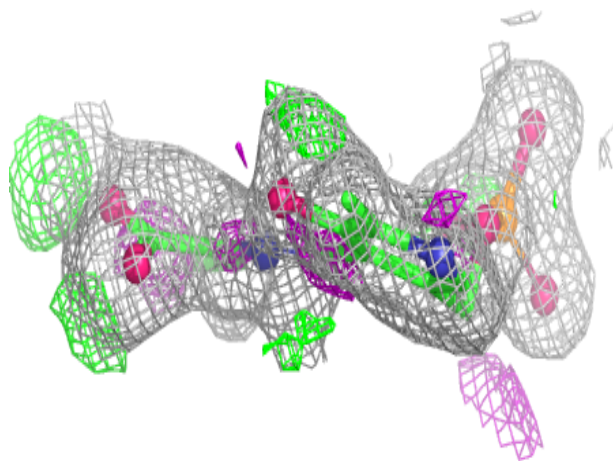
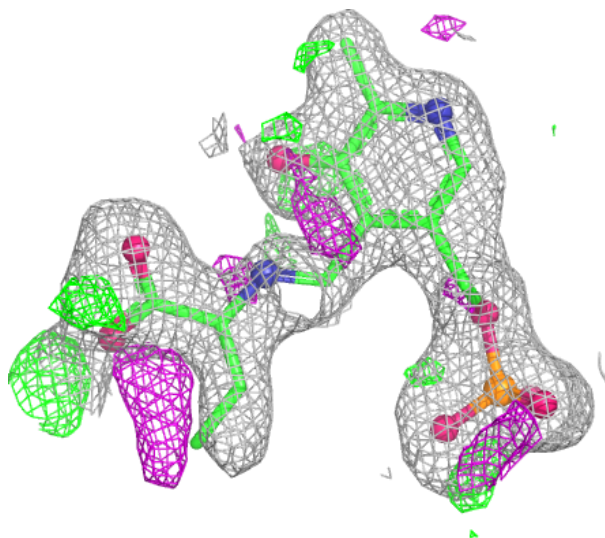
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HCS	C	501	8/8	0.66	0.24	60,63,64,76	0
3	HCS	A	501	8/8	0.70	0.22	58,63,69,79	0
5	H2S	B	402	1/1	0.86	0.13	74,74,74,74	0
4	4LM	B	401	22/22	0.94	0.11	19,32,47,50	0
6	7XF	D	501	23/23	0.94	0.12	16,26,54,71	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.

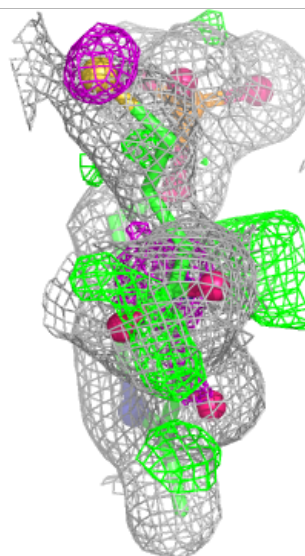
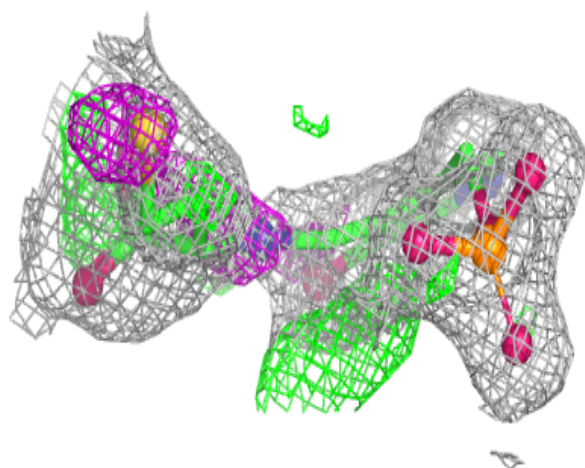
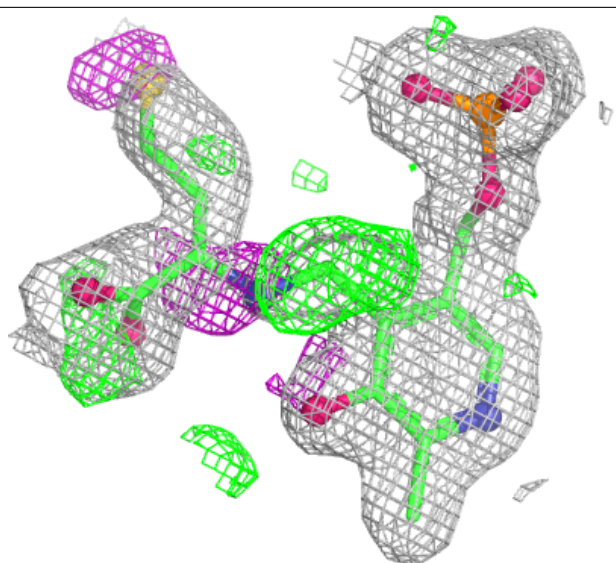
Electron density around 4LM B 401:

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



Electron density around 7XF D 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.