Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 10:14 am GMT

PDB ID	:	6EVE
Title	:	Structure of R175A S. cerevisiae Fdc1 with prFMN in the iminium form
Authors	:	Bailey, S.S.; David, L.
Deposited on	:	2017-11-01
Resolution	:	2.05 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 (i) 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 (i)) were used in the production of this report:

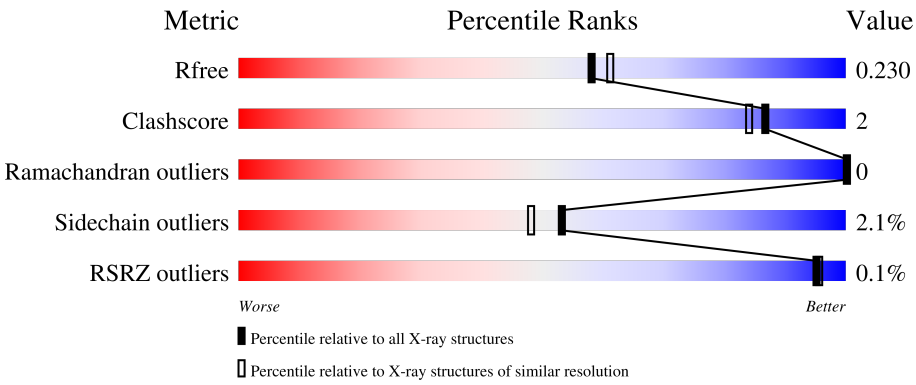
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	509	92% 6% •
1	B	509	91% 7% • •
1	C	509	91% 7% •
1	D	509	90% 7% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17196 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 Ferulic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	500	3976	2558	648	745	25	0	11	0
1	B	499	3941	2537	639	742	23	0	9	0
1	C	500	3951	2543	642	742	24	0	10	0
1	D	497	3931	2534	636	737	24	0	9	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	ALA	ARG	engineered mutation	UNP Q03034
A	504	HIS	-	expression tag	UNP Q03034
A	505	HIS	-	expression tag	UNP Q03034
A	506	HIS	-	expression tag	UNP Q03034
A	507	HIS	-	expression tag	UNP Q03034
A	508	HIS	-	expression tag	UNP Q03034
A	509	HIS	-	expression tag	UNP Q03034
B	175	ALA	ARG	engineered mutation	UNP Q03034
B	504	HIS	-	expression tag	UNP Q03034
B	505	HIS	-	expression tag	UNP Q03034
B	506	HIS	-	expression tag	UNP Q03034
B	507	HIS	-	expression tag	UNP Q03034
B	508	HIS	-	expression tag	UNP Q03034
B	509	HIS	-	expression tag	UNP Q03034
C	175	ALA	ARG	engineered mutation	UNP Q03034
C	504	HIS	-	expression tag	UNP Q03034
C	505	HIS	-	expression tag	UNP Q03034
C	506	HIS	-	expression tag	UNP Q03034
C	507	HIS	-	expression tag	UNP Q03034
C	508	HIS	-	expression tag	UNP Q03034
C	509	HIS	-	expression tag	UNP Q03034

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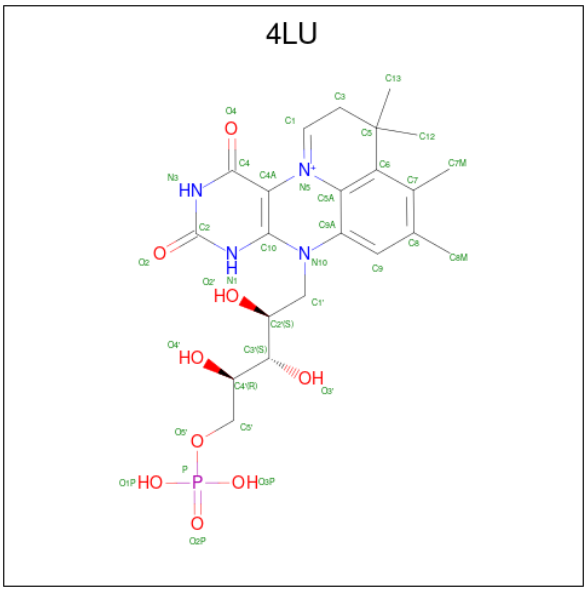
Chain	Residue	Modelled	Actual	Comment	Reference
D	175	ALA	ARG	engineered mutation	UNP Q03034
D	504	HIS	-	expression tag	UNP Q03034
D	505	HIS	-	expression tag	UNP Q03034
D	506	HIS	-	expression tag	UNP Q03034
D	507	HIS	-	expression tag	UNP Q03034
D	508	HIS	-	expression tag	UNP Q03034
D	509	HIS	-	expression tag	UNP Q03034

- Molecule 2 is 1-deoxy-5-O-phosphono-1-(3,3,4,5-tetramethyl-9,11-dioxo-2,3,8,9,10,11-hexah ydro-7H-quinolino[1,8-fg]pteridin-12-ium-7-y l)-D-ribitol (three-letter code: 4LU) (formula: $C_{22}H_{30}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	22	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			36	22	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			36	22	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			36	22	4	9	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	2	2	2	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0

- Molecule 5 is water.

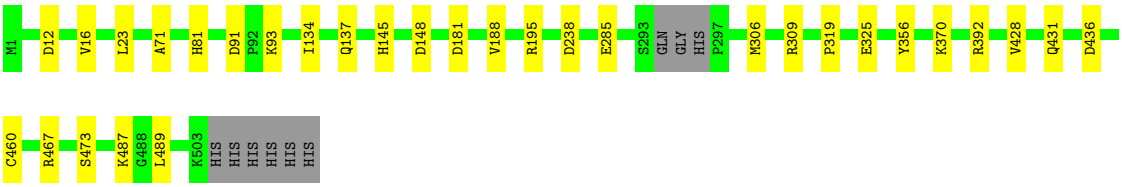
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	323	323	323	0	0
5	B	317	317	317	0	0
5	C	356	356	356	0	0
5	D	249	249	249	0	0

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.

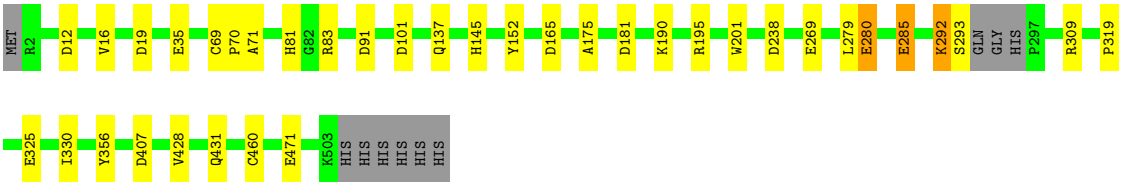
• Molecule 1: Ferulic acid decarboxylase 1

Chain A:



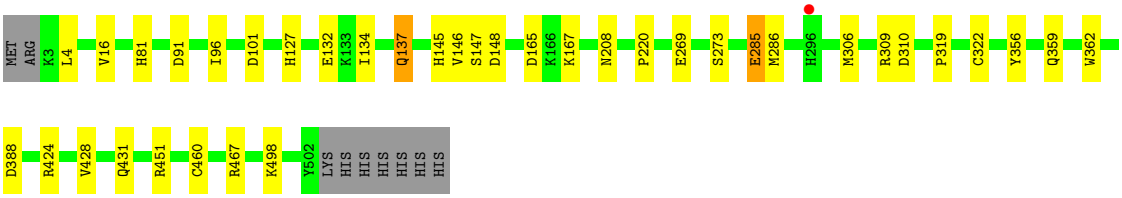
• Molecule 1: Ferulic acid decarboxylase 1

Chain B:



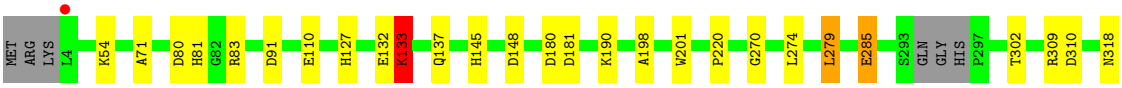
• Molecule 1: Ferulic acid decarboxylase 1

Chain C:



• Molecule 1: Ferulic acid decarboxylase 1

Chain D:



P319
C322
E325
E344
Y356
Q359
G387
R392
V428
Q431
F434
C460
K503
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.48Å 98.64Å 118.17Å 90.00° 97.24° 90.00°	Depositor
Resolution (Å)	77.89 – 2.05 77.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (77.89-2.05) 99.7 (77.89-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.183 , 0.226 0.191 , 0.230	Depositor DCC
R_{free} test set	8336 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17196	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, 4LU, K

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	0.89	0/4074	0.90	4/5534 (0.1%)
1	B	0.98	5/4039 (0.1%)	0.93	13/5490 (0.2%)
1	C	0.87	1/4051 (0.0%)	0.92	9/5512 (0.2%)
1	D	0.88	2/4029 (0.0%)	0.89	10/5477 (0.2%)
All	All	0.90	8/16193 (0.0%)	0.91	36/22013 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	GLU	N-CA	-14.44	1.17	1.46
1	B	280	GLU	N-CA	-12.26	1.21	1.46
1	B	175	ALA	N-CA	-9.97	1.26	1.46
1	B	175	ALA	CA-C	-8.21	1.31	1.52
1	D	201	TRP	CE3-CZ3	5.74	1.48	1.38
1	D	344	GLU	CD-OE2	5.59	1.31	1.25
1	B	201	TRP	CE3-CZ3	5.57	1.48	1.38
1	C	362	TRP	CE3-CZ3	5.17	1.47	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	195	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	467	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	B	195	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	D	83	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	309	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	91	ASP	CB-CG-OD1	7.05	124.65	118.30
1	C	91	ASP	CB-CG-OD1	6.73	124.35	118.30
1	B	309	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	C	309	ARG	NE-CZ-NH1	6.50	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	83	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	407	ASP	CB-CG-OD1	6.34	124.01	118.30
1	B	292	LYS	N-CA-C	6.30	128.02	111.00
1	B	101	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	388	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	285	GLU	N-CA-CB	-5.89	100.00	110.60
1	D	309	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	91	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	83	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	309	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	451	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	424	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	D	91	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	285	GLU	CB-CA-C	5.44	121.27	110.40
1	B	83	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	C	165	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	133	LYS	CD-CE-NZ	5.33	123.96	111.70
1	B	19	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	392	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	101	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	309	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	238	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	238	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	285	GLU	CA-CB-CG	5.19	124.82	113.40
1	D	180	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	165	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	424	ARG	NE-CZ-NH1	5.07	122.84	120.30

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	3976	0	3954	13	0
1	B	3941	0	3903	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3951	0	3907	17	0
1	D	3931	0	3906	18	0
2	A	36	0	28	2	0
2	B	36	0	26	4	0
2	C	36	0	28	2	0
2	D	36	0	28	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	323	0	0	1	0
5	B	317	0	0	1	0
5	C	356	0	0	3	0
5	D	249	0	0	2	0
All	All	17196	0	15780	68	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 (68) 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)
2:D:601:4LU:H5	2:D:601:4LU:H14	1.33	1.08
2:A:601:4LU:H5	2:A:601:4LU:H14	1.40	1.03
2:C:601:4LU:H14	2:C:601:4LU:H5	1.40	1.02
2:B:601:4LU:H14	2:B:601:4LU:H5	1.43	0.99
2:D:601:4LU:H14	2:D:601:4LU:C13	2.06	0.85
2:A:601:4LU:H14	2:A:601:4LU:C13	2.08	0.83
2:B:601:4LU:H14	2:B:601:4LU:C13	2.10	0.81
1:C:498:LYS:CA	5:C:1002:HOH:O	2.31	0.77
2:C:601:4LU:H14	2:C:601:4LU:C13	2.16	0.76
1:C:322:CYS:H	1:C:359:GLN:HE22	1.34	0.75
1:A:428:VAL:H	1:A:431:GLN:HE21	1.37	0.73
1:A:81:HIS:HE1	1:A:356:TYR:OH	1.77	0.67
1:D:81:HIS:HE1	1:D:356:TYR:OH	1.77	0.66
1:C:145:HIS:HE1	1:C:319:PRO:O	1.85	0.59
1:D:133:LYS:HA	1:D:133:LYS:CE	2.33	0.58
1:B:81:HIS:HE1	1:B:356:TYR:OH	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ALA:HB3	1:A:325:GLU:HG3	1.86	0.56
1:C:81:HIS:HE1	1:C:356:TYR:OH	1.89	0.56
1:C:428:VAL:H	1:C:431:GLN:HE21	1.51	0.56
1:D:71:ALA:HB3	1:D:325:GLU:HG3	1.87	0.56
1:D:133:LYS:HA	1:D:133:LYS:HE3	1.88	0.56
1:B:428:VAL:H	1:B:431:GLN:HE21	1.54	0.55
1:D:428:VAL:H	1:D:431:GLN:HE21	1.53	0.55
1:B:152:TYR:OH	1:B:280:GLU:OE2	2.24	0.53
1:B:145:HIS:HE1	1:B:319:PRO:O	1.92	0.53
1:A:12:ASP:O	1:A:16[B]:VAL:HG13	2.09	0.52
1:A:145:HIS:HE1	1:A:319:PRO:O	1.93	0.52
1:D:428:VAL:H	1:D:431:GLN:NE2	2.07	0.52
1:C:208[A]:ASN:ND2	1:C:273:SER:OG	2.43	0.51
1:D:145:HIS:HD2	1:D:148:ASP:OD2	1.94	0.50
1:D:322:CYS:H	1:D:359:GLN:HE22	1.60	0.49
1:C:127:HIS:HE1	1:C:310:ASP:OD1	1.95	0.49
1:C:467:ARG:HD3	5:C:859:HOH:O	2.13	0.48
1:A:134:ILE:HD13	1:A:306[B]:MET:HE3	1.96	0.48
1:B:293:SER:HB2	5:B:964:HOH:O	2.14	0.47
1:C:428:VAL:H	1:C:431:GLN:NE2	2.11	0.47
1:A:436[B]:ASP:OD1	1:A:436[B]:ASP:C	2.54	0.46
1:C:137:GLN:NE2	5:C:711:HOH:O	2.49	0.46
1:D:145:HIS:CE1	1:D:318:ASN:OD1	2.69	0.45
2:D:601:4LU:C13	2:D:601:4LU:C7M	2.86	0.45
1:C:134:ILE:HD12	1:C:306[B]:MET:HE3	1.97	0.45
1:D:279:LEU:HD22	5:D:865:HOH:O	2.16	0.45
1:C:96[A]:ILE:O	1:C:96[A]:ILE:HG13	2.17	0.45
1:C:285:GLU:HG2	1:C:286:MET:N	2.31	0.45
1:A:428:VAL:H	1:A:431:GLN:NE2	2.10	0.45
1:C:145:HIS:HD2	1:C:148:ASP:OD2	2.00	0.44
1:C:4:LEU:HD13	1:C:16[B]:VAL:HG12	2.00	0.44
1:D:387:GLY:HA3	1:D:434:PHE:CZ	2.53	0.43
1:D:127:HIS:HE1	1:D:310:ASP:OD1	2.01	0.43
1:D:198:ALA:HB1	1:D:274:LEU:HD11	1.99	0.43
1:C:146:VAL:O	1:C:147:SER:HB2	2.18	0.43
1:A:145:HIS:HD2	1:A:148:ASP:OD2	2.02	0.43
1:A:188:VAL:O	1:A:195:ARG:HD3	2.19	0.42
1:D:80:ASP:OD1	1:D:81:HIS:HD2	2.01	0.42
1:A:489:LEU:HD11	1:B:35:GLU:HG3	2.00	0.42
1:D:145:HIS:HE1	1:D:319:PRO:O	2.01	0.42
1:B:71:ALA:HB3	1:B:325:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436[B]:ASP:OD1	1:A:436[B]:ASP:O	2.36	0.42
1:B:69:CYS:N	1:B:70:PRO:CD	2.82	0.41
1:B:16[A]:VAL:O	1:B:16[A]:VAL:HG22	2.19	0.41
1:A:370[B]:LYS:HG2	5:A:890:HOH:O	2.21	0.41
2:B:601:4LU:H7	2:B:601:4LU:H22	1.84	0.41
1:B:330:ILE:HD11	2:B:601:4LU:C9A	2.51	0.41
1:B:12:ASP:O	1:B:16[B]:VAL:HG13	2.20	0.41
1:D:133:LYS:HA	1:D:133:LYS:HE2	2.02	0.41
1:D:190:LYS:HD3	5:D:841:HOH:O	2.21	0.41
1:D:270:GLY:HA3	1:D:302:THR:O	2.22	0.40
1:C:306[B]:MET:HE2	1:C:306[B]:MET:HB2	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/509 (100%)	492 (97%)	15 (3%)	0	100	100
1	B	504/509 (99%)	492 (98%)	12 (2%)	0	100	100
1	C	508/509 (100%)	495 (97%)	13 (3%)	0	100	100
1	D	501/509 (98%)	487 (97%)	14 (3%)	0	100	100
All	All	2020/2036 (99%)	1966 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/443 (99%)	429 (98%)	11 (2%)	47	40
1	B	435/443 (98%)	426 (98%)	9 (2%)	53	48
1	C	436/443 (98%)	428 (98%)	8 (2%)	59	55
1	D	435/443 (98%)	424 (98%)	11 (2%)	47	40
All	All	1746/1772 (98%)	1707 (98%)	39 (2%)	53	46

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	93	LYS
1	A	137	GLN
1	A	181	ASP
1	A	285	GLU
1	A	392	ARG
1	A	460[A]	CYS
1	A	460[B]	CYS
1	A	473[A]	SER
1	A	473[B]	SER
1	A	487	LYS
1	B	137	GLN
1	B	181	ASP
1	B	190	LYS
1	B	269	GLU
1	B	279	LEU
1	B	285	GLU
1	B	292	LYS
1	B	460	CYS
1	B	471	GLU
1	C	132	GLU
1	C	137	GLN
1	C	167	LYS
1	C	220	PRO
1	C	269	GLU
1	C	285	GLU
1	C	460[A]	CYS
1	C	460[B]	CYS
1	D	54	LYS
1	D	110	GLU

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Mol	Chain	Res	Type
1	D	132	GLU
1	D	133	LYS
1	D	137	GLN
1	D	181	ASP
1	D	220	PRO
1	D	279	LEU
1	D	285	GLU
1	D	460[A]	CYS
1	D	460[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	127	HIS
1	A	145	HIS
1	A	431	GLN
1	A	448	GLN
1	B	81	HIS
1	B	127	HIS
1	B	145	HIS
1	B	431	GLN
1	B	448	GLN
1	C	81	HIS
1	C	127	HIS
1	C	145	HIS
1	C	359	GLN
1	C	431	GLN
1	D	81	HIS
1	D	127	HIS
1	D	137	GLN
1	D	145	HIS
1	D	359	GLN
1	D	431	GLN
1	D	496	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - 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	$\#\|Z\| > 2$
2	4LU	C	601	3,4	35,39,39	1.67	4 (11%)	46,62,62	2.27	14 (30%)
2	4LU	B	601	3,4	35,39,39	3.11	8 (22%)	46,62,62	2.32	15 (32%)
2	4LU	D	601	3	35,39,39	1.67	4 (11%)	46,62,62	2.23	17 (36%)
2	4LU	A	601	3,4	35,39,39	1.84	5 (14%)	46,62,62	2.02	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4LU	C	601	3,4	-	0/18/30/30	0/4/4/4
2	4LU	B	601	3,4	-	2/18/30/30	0/4/4/4
2	4LU	D	601	3	-	1/18/30/30	0/4/4/4
2	4LU	A	601	3,4	-	2/18/30/30	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	4LU	C1'-N10	-15.01	1.10	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	4LU	O2-C2	6.36	1.36	1.23
2	B	601	4LU	O2-C2	5.88	1.35	1.23
2	C	601	4LU	O2-C2	5.85	1.35	1.23
2	A	601	4LU	O2-C2	5.79	1.35	1.23
2	A	601	4LU	C3-C5	-5.38	1.46	1.54
2	C	601	4LU	C3-C5	-4.98	1.46	1.54
2	B	601	4LU	C1'-C2'	4.27	1.58	1.52
2	D	601	4LU	C3-C5	-4.13	1.48	1.54
2	B	601	4LU	C3-C5	-4.02	1.48	1.54
2	B	601	4LU	C5A-C6	3.13	1.42	1.39
2	A	601	4LU	C4A-C10	2.97	1.45	1.39
2	A	601	4LU	C9-C8	-2.66	1.35	1.39
2	B	601	4LU	C10-N10	2.56	1.43	1.38
2	D	601	4LU	C5'-C4'	2.51	1.55	1.51
2	B	601	4LU	C8M-C8	-2.42	1.46	1.51
2	C	601	4LU	C10-N10	2.30	1.42	1.38
2	C	601	4LU	P-O3P	-2.26	1.46	1.54
2	A	601	4LU	O4-C4	2.23	1.27	1.23
2	D	601	4LU	C5A-C6	2.11	1.41	1.39
2	B	601	4LU	C5'-C4'	2.01	1.54	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	4LU	C4-C4A-C10	-7.77	114.84	121.08
2	B	601	4LU	C4-C4A-C10	-6.98	115.47	121.08
2	D	601	4LU	C5-C6-C5A	-6.12	114.80	121.48
2	A	601	4LU	C4-C4A-C10	-5.93	116.32	121.08
2	D	601	4LU	C4-C4A-C10	-5.84	116.39	121.08
2	C	601	4LU	C5-C6-C5A	-5.54	115.43	121.48
2	B	601	4LU	C5-C6-C5A	-5.48	115.50	121.48
2	B	601	4LU	C1'-C2'-C3'	4.96	123.64	109.79
2	B	601	4LU	C4A-C4-N3	4.91	122.04	111.79
2	C	601	4LU	C4A-C4-N3	4.88	121.98	111.79
2	D	601	4LU	C4A-C4-N3	4.51	121.22	111.79
2	D	601	4LU	C4-N3-C2	-4.22	120.25	126.34
2	A	601	4LU	N1-C2-N3	4.07	122.35	115.80
2	C	601	4LU	C13-C5-C3	-3.92	102.81	109.60
2	B	601	4LU	C4-N3-C2	-3.91	120.70	126.34
2	A	601	4LU	C5-C6-C5A	-3.82	117.31	121.48
2	A	601	4LU	C9-C8-C7	3.62	123.17	119.18
2	C	601	4LU	C4-N3-C2	-3.52	121.27	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	4LU	C4A-C4-N3	3.45	119.00	111.79
2	D	601	4LU	P-O5'-C5'	3.28	127.32	118.30
2	D	601	4LU	C13-C5-C3	-3.21	104.03	109.60
2	A	601	4LU	C1'-N10-C9A	3.20	125.85	120.51
2	D	601	4LU	O1P-P-O5'	3.19	115.23	106.73
2	D	601	4LU	C8M-C8-C7	3.14	126.05	121.17
2	A	601	4LU	C4-N3-C2	-3.13	121.83	126.34
2	D	601	4LU	C8M-C8-C9	-3.05	113.85	119.49
2	C	601	4LU	O4-C4-N3	-3.04	114.28	120.12
2	B	601	4LU	C1'-N10-C9A	2.92	125.38	120.51
2	A	601	4LU	C8M-C8-C9	-2.77	114.37	119.49
2	B	601	4LU	C13-C5-C3	-2.74	104.86	109.60
2	B	601	4LU	O5'-P-O2P	-2.68	98.95	106.47
2	D	601	4LU	C3-C5-C6	2.67	113.47	107.38
2	D	601	4LU	O1P-P-O3P	2.66	117.81	107.64
2	A	601	4LU	O1P-P-O3P	2.64	117.71	107.64
2	B	601	4LU	O4-C4-N3	-2.64	115.06	120.12
2	C	601	4LU	C8M-C8-C9	-2.59	114.71	119.49
2	C	601	4LU	N1-C2-N3	2.55	119.91	115.80
2	B	601	4LU	O1P-P-O3P	2.50	117.17	107.64
2	B	601	4LU	O2'-C2'-C3'	-2.48	103.08	109.10
2	B	601	4LU	C9-C8-C7	2.46	121.89	119.18
2	C	601	4LU	C1'-N10-C9A	2.46	124.61	120.51
2	C	601	4LU	O1P-P-O3P	2.44	116.97	107.64
2	D	601	4LU	O4-C4-N3	-2.44	115.44	120.12
2	D	601	4LU	C12-C5-C3	-2.42	105.41	109.60
2	A	601	4LU	C13-C5-C3	-2.40	105.44	109.60
2	C	601	4LU	C9-C8-C7	2.39	121.81	119.18
2	D	601	4LU	C4'-C3'-C2'	-2.35	108.47	113.36
2	B	601	4LU	O4-C4-C4A	-2.32	122.83	128.06
2	B	601	4LU	C4'-C3'-C2'	2.29	118.12	113.36
2	D	601	4LU	N1-C2-N3	2.28	119.47	115.80
2	A	601	4LU	O4-C4-N3	-2.22	115.86	120.12
2	D	601	4LU	O4-C4-C4A	-2.10	123.33	128.06
2	A	601	4LU	O3P-P-O5'	-2.10	101.16	106.73
2	B	601	4LU	O2'-C2'-C1'	-2.09	104.74	109.80
2	D	601	4LU	O5'-P-O2P	-2.07	100.66	106.47
2	C	601	4LU	C7M-C7-C8	-2.07	115.89	119.71
2	C	601	4LU	O5'-C5'-C4'	-2.07	103.84	109.36
2	C	601	4LU	P-O5'-C5'	2.05	123.95	118.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	4LU	C2'-C3'-C4'-C5'
2	B	601	4LU	C2'-C3'-C4'-C5'
2	A	601	4LU	C4'-C5'-O5'-P
2	D	601	4LU	C4'-C5'-O5'-P
2	B	601	4LU	C4'-C5'-O5'-P

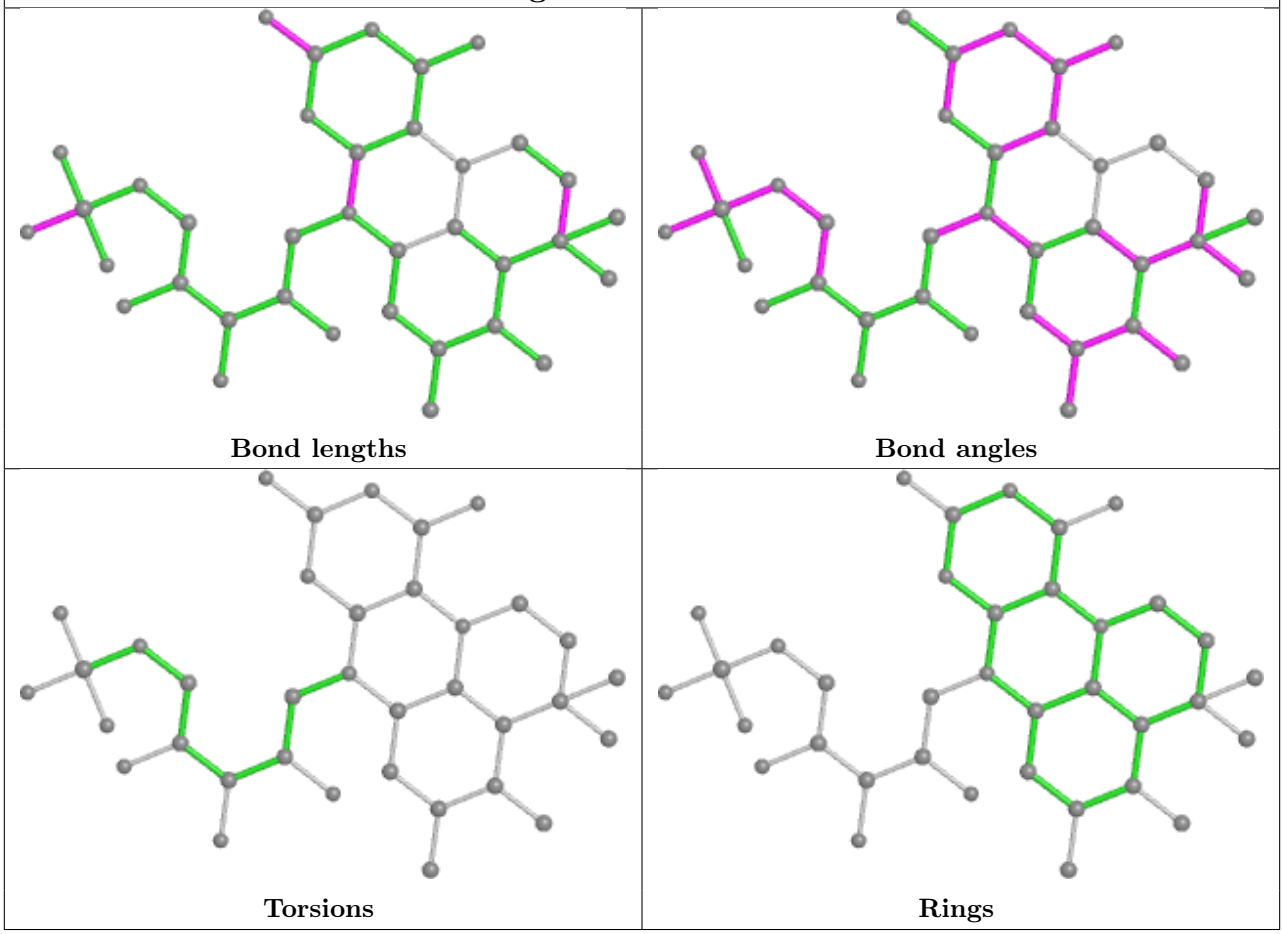
There are no ring outliers.

4 monomers are involved in 11 short contacts:

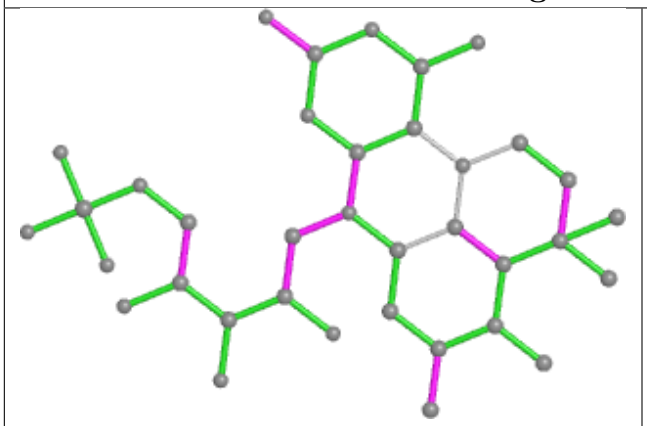
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	4LU	2	0
2	B	601	4LU	4	0
2	D	601	4LU	3	0
2	A	601	4LU	2	0

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 then 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.

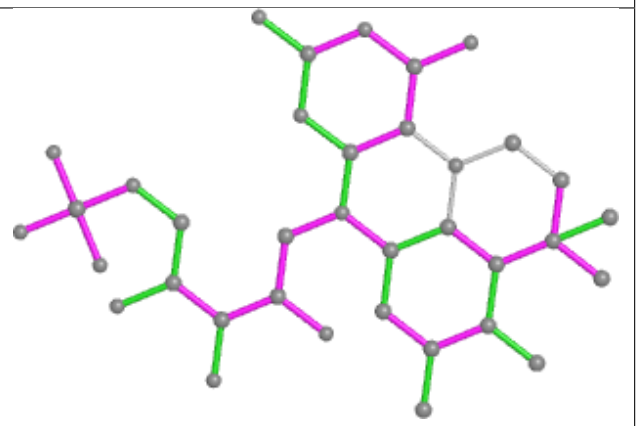
Ligand 4LU C 601



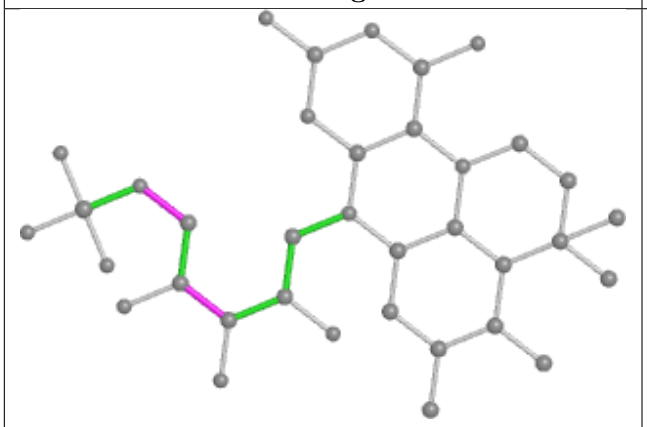
Ligand 4LU B 601



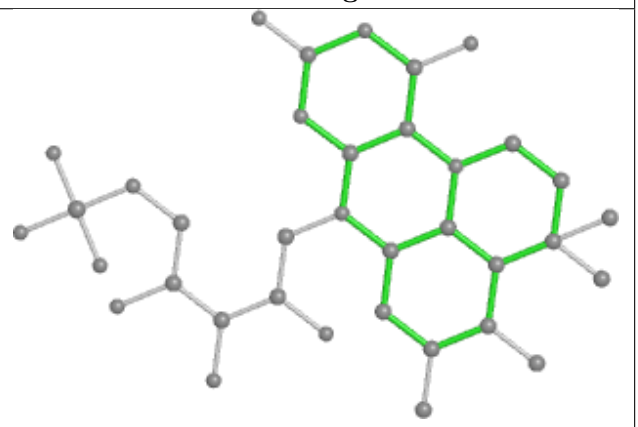
Bond lengths



Bond angles

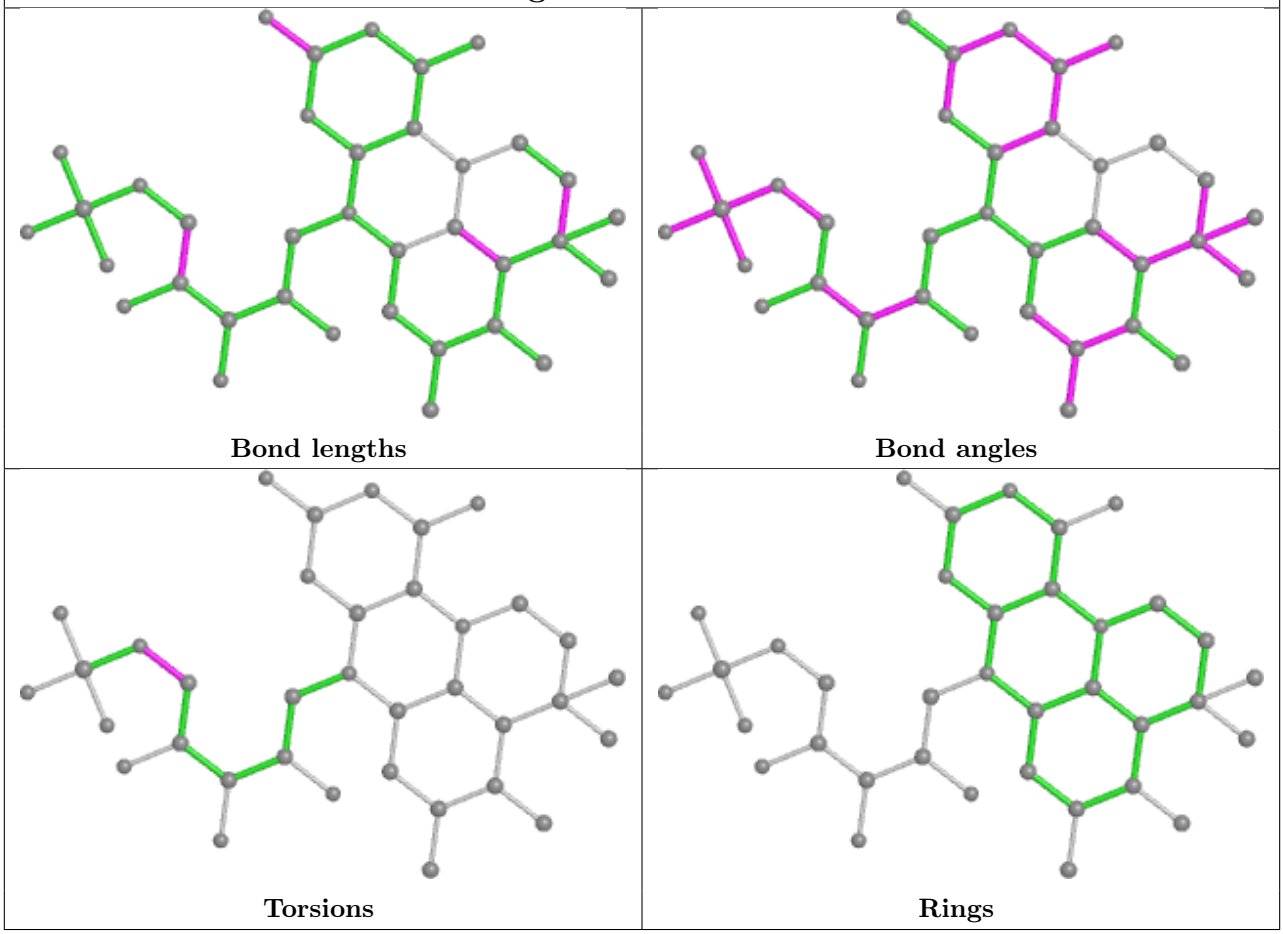


Torsions

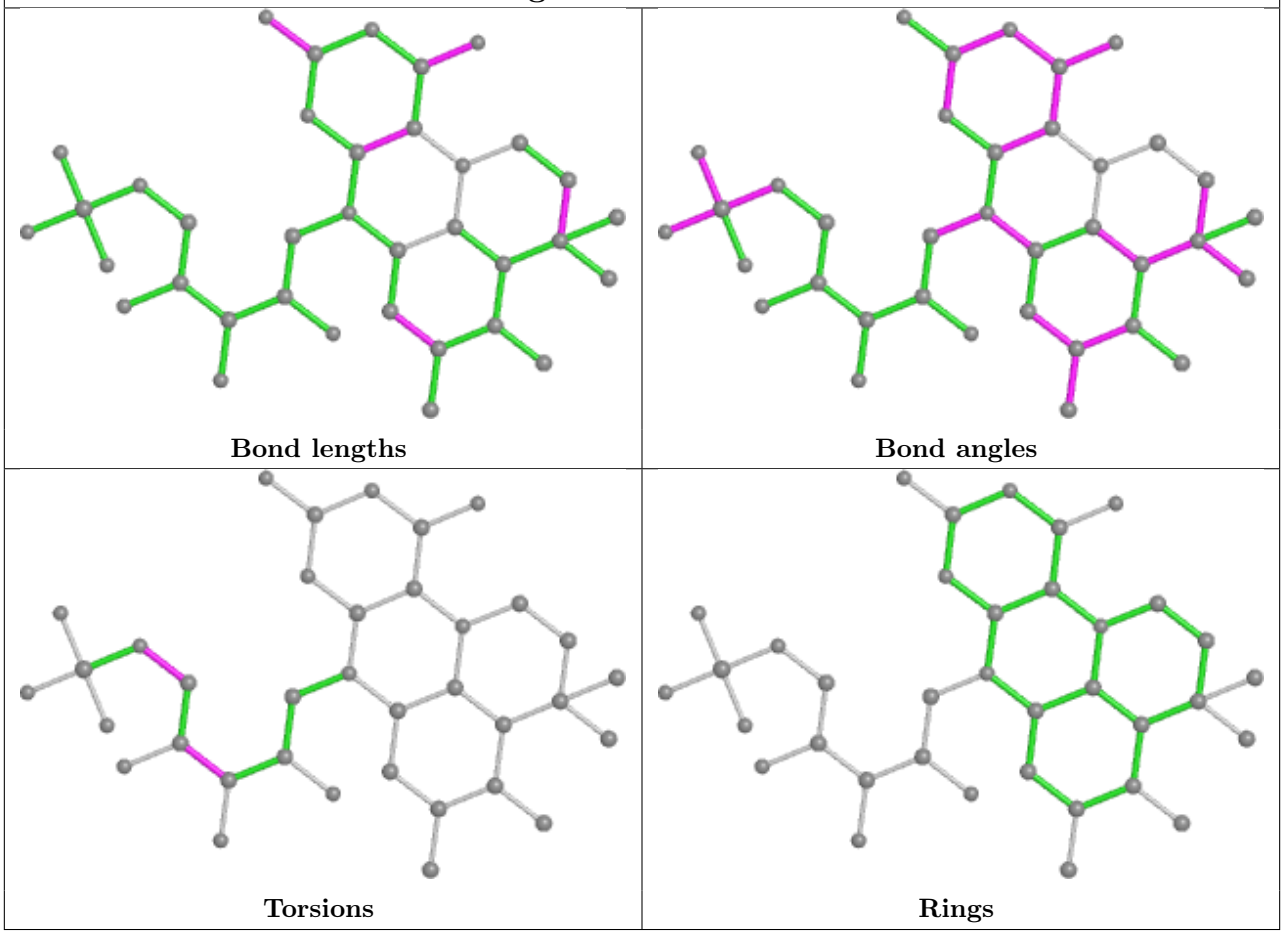


Rings

Ligand 4LU D 601



Ligand 4LU A 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	500/509 (98%)	-0.58	0	100	100	16, 23, 39, 57	0
1	B	499/509 (98%)	-0.65	0	100	100	17, 26, 44, 65	0
1	C	500/509 (98%)	-0.59	1 (0%)	95	95	16, 25, 43, 58	2 (0%)
1	D	497/509 (97%)	-0.62	1 (0%)	95	95	18, 28, 43, 64	0
All	All	1996/2036 (98%)	-0.61	2 (0%)	95	95	16, 26, 43, 65	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	HIS	3.3
1	D	4[A]	LEU	2.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

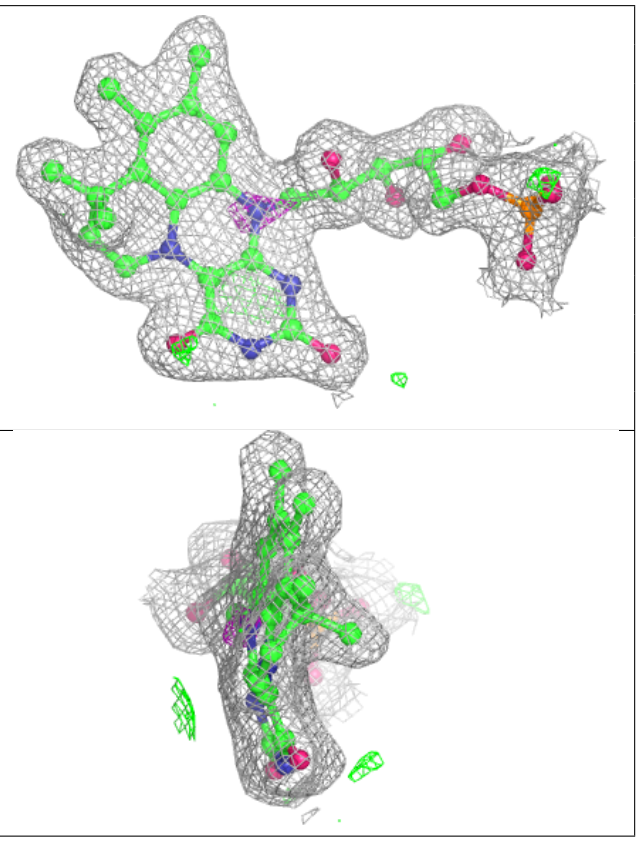
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4LU	B	601	36/36	0.96	0.09	15,18,22,25	0
2	4LU	A	601	36/36	0.97	0.10	15,17,22,28	0
2	4LU	D	601	36/36	0.97	0.09	16,22,25,26	0
2	4LU	C	601	36/36	0.98	0.09	15,20,27,31	0
3	MN	D	603	1/1	0.99	0.05	32,32,32,32	0
4	K	A	603	1/1	0.99	0.11	18,18,18,18	0
4	K	B	603	1/1	0.99	0.09	21,21,21,21	0
4	K	C	603	1/1	0.99	0.09	19,19,19,19	0
3	MN	A	602	1/1	1.00	0.09	24,24,24,24	0
3	MN	B	602	1/1	1.00	0.07	27,27,27,27	0
3	MN	C	602	1/1	1.00	0.07	24,24,24,24	0
3	MN	D	602	1/1	1.00	0.08	24,24,24,24	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.

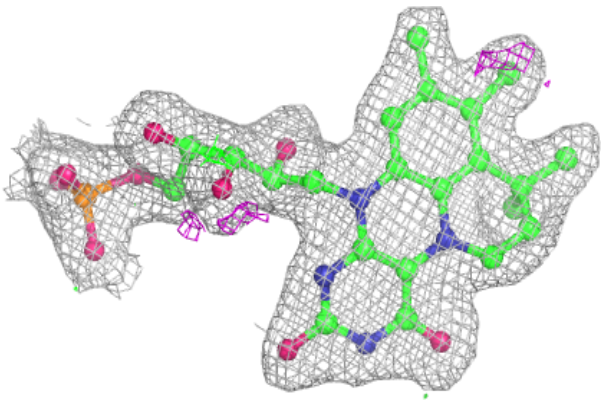
Electron density around 4LU B 601:

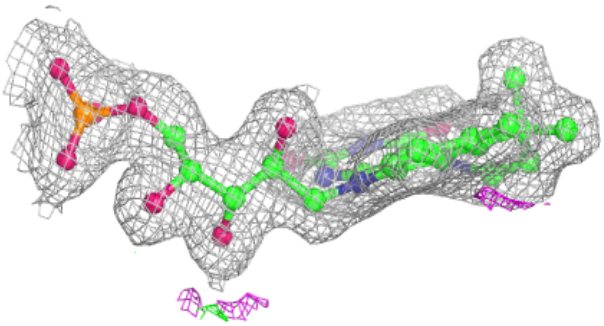
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 4LU A 601:

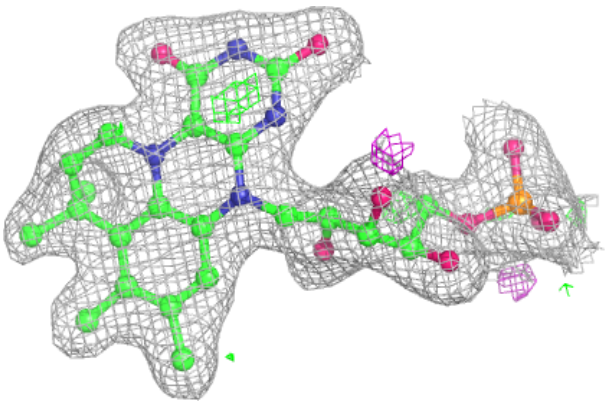
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

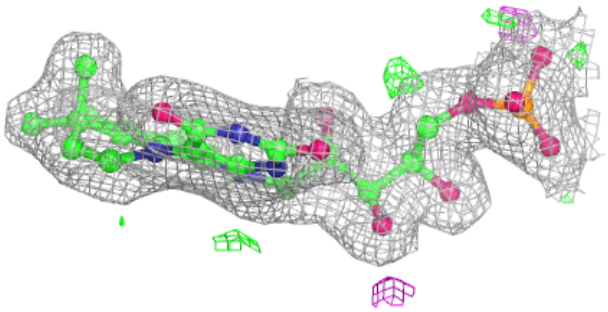


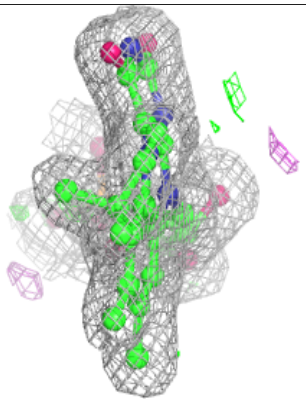


Electron density around 4LU D 601:

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

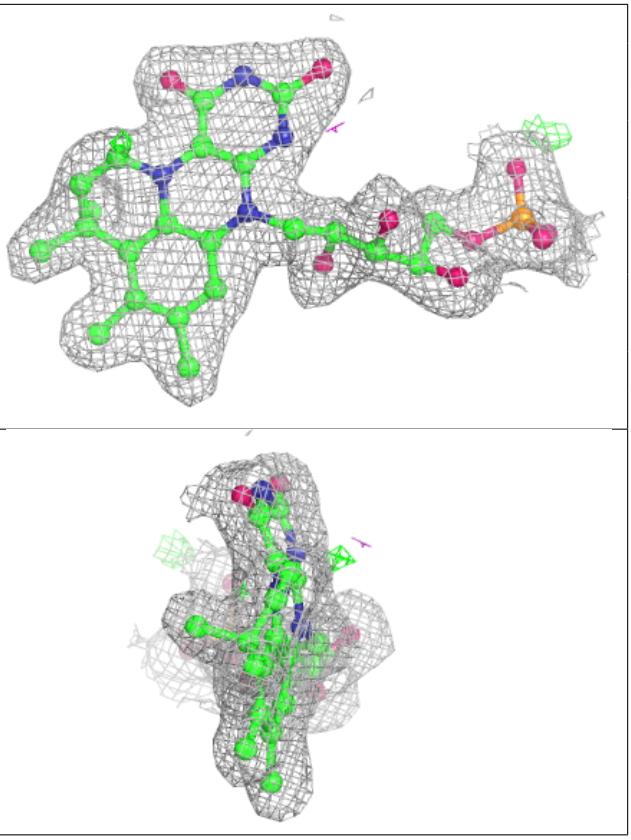


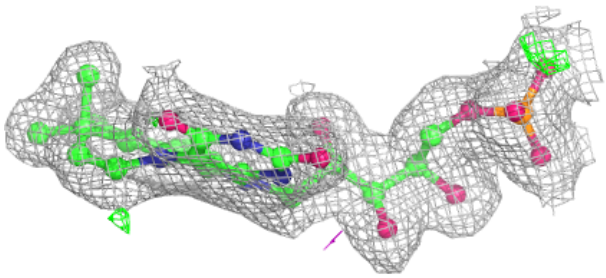




Electron density around 4LU C 601:

$2mF_o$-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.