



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:23 pm BST

PDB ID : 4ZAC  
Title : Structure of *S. cerevisiae* Fdc1 with the prenylated-flavin cofactor in the iminium form.  
Authors : White, M.D.; Leys, D.  
Deposited on : 2015-04-13  
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

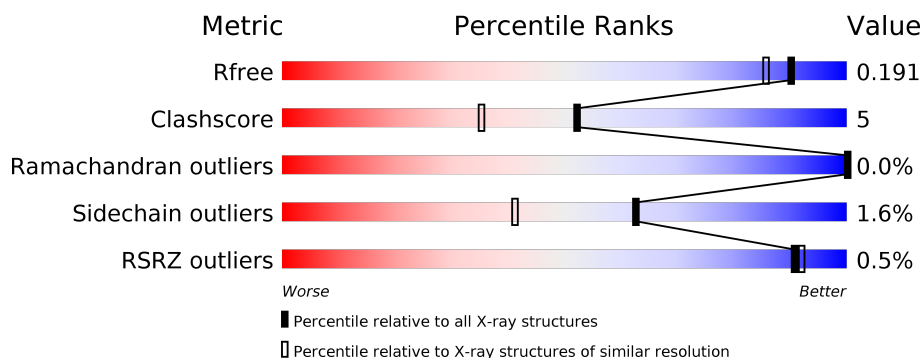
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	503	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>14%</span> <span>.</span> </div> </div>
1	B	503	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 15%, green 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>84%</span> <span>15%</span> <span>.</span> </div> </div>
1	C	503	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 17%, green 82%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>82%</span> <span>17%</span> <span>.</span> </div> </div>
1	D	503	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 86%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>13%</span> <span>.</span> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17693 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
1	A	503	Total	C	N	O	S	0	14	0
			4052	2604	667	756	25			
1	B	503	Total	C	N	O	S	0	11	0
			4032	2594	659	755	24			
1	C	501	Total	C	N	O	S	0	9	0
			3975	2560	648	743	24			
1	D	503	Total	C	N	O	S	0	12	0
			4032	2593	658	755	26			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

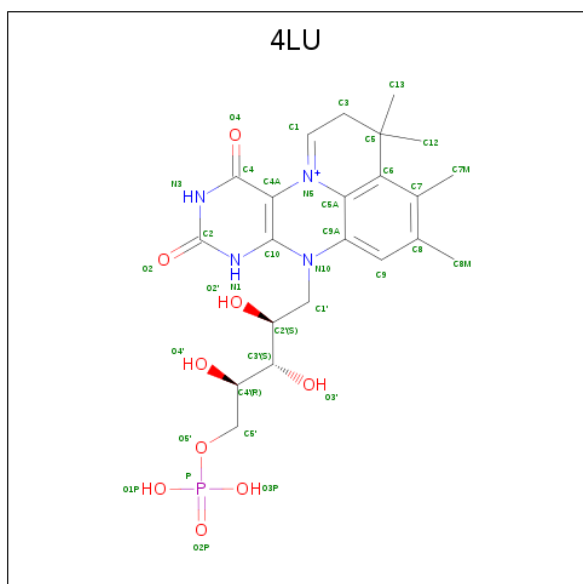
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	437	Total O 437 437	0	0

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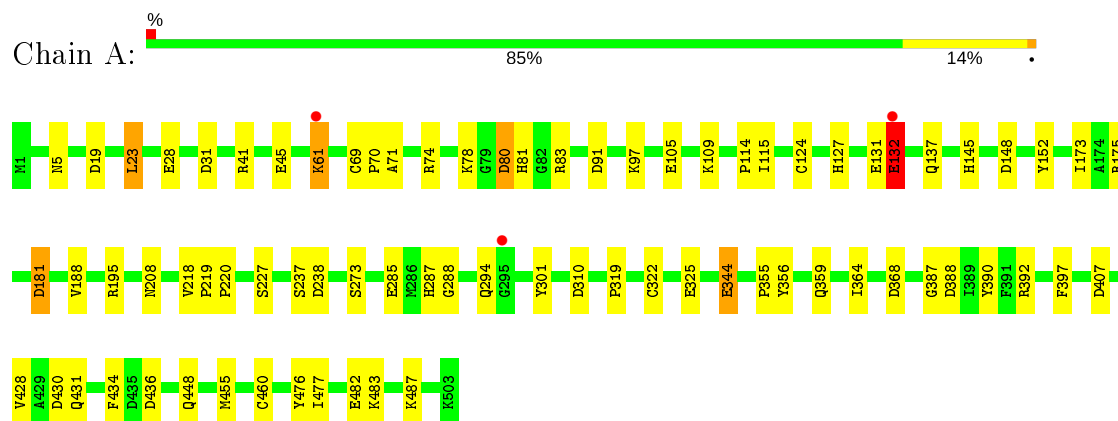
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	358	Total 358	O 358	0	0
6	C	275	Total 275	O 275	0	0
6	D	377	Total 377	O 377	0	0

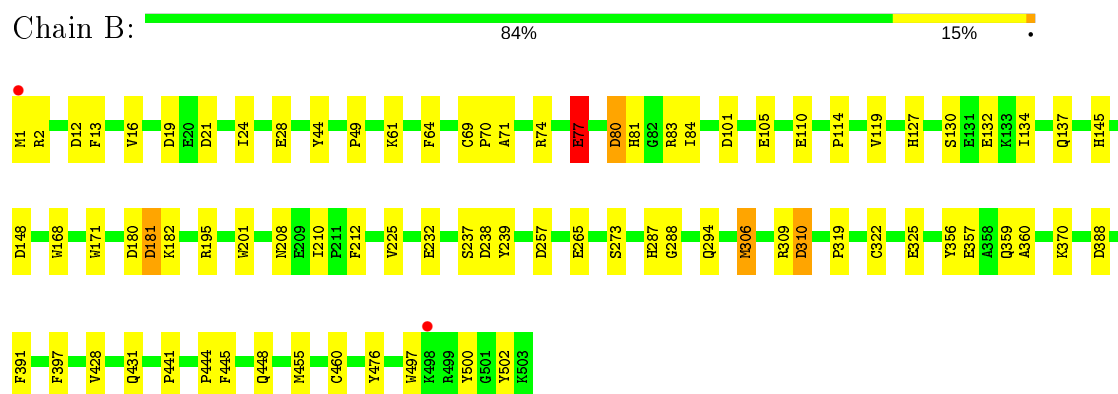
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

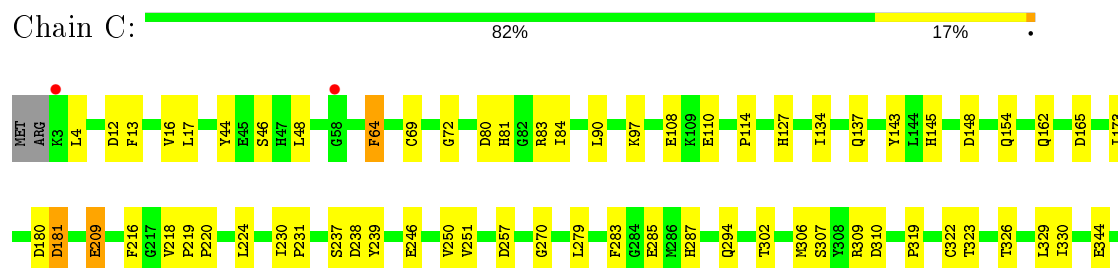
#### • Molecule 1: Ferulic acid decarboxylase 1



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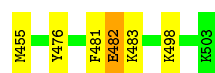
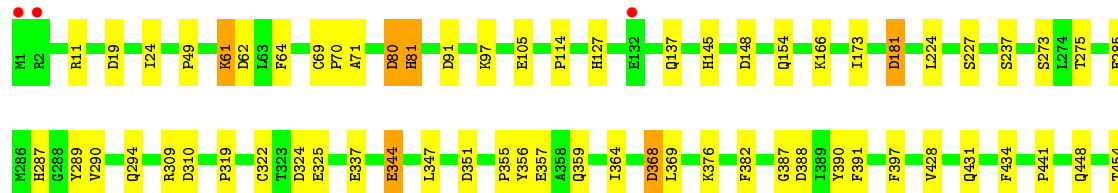
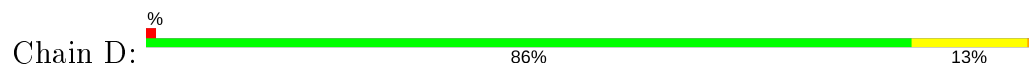


#### • Molecule 1: Ferulic acid decarboxylase 1





• Molecule 1: Ferulic acid decarboxylase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.41Å 96.18Å 116.64Å 90.00° 96.58° 90.00°	Depositor
Resolution (Å)	54.19 – 1.65 54.19 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.19-1.65) 98.7 (54.19-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.163 , 0.192 0.161 , 0.191	Depositor DCC
$R_{free}$ test set	15010 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, MN, 4LU

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	1.49	15/4152 (0.4%)	1.32	21/5637 (0.4%)
1	B	1.46	20/4133 (0.5%)	1.30	25/5612 (0.4%)
1	C	1.49	19/4078 (0.5%)	1.29	19/5542 (0.3%)
1	D	1.43	15/4132 (0.4%)	1.26	21/5611 (0.4%)
All	All	1.47	69/16495 (0.4%)	1.29	86/22402 (0.4%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	482	GLU	CG-CD	9.18	1.65	1.51
1	C	69	CYS	CB-SG	-8.50	1.67	1.82
1	A	301	TYR	CD2-CE2	7.54	1.50	1.39
1	A	344	GLU	CG-CD	7.47	1.63	1.51
1	A	482	GLU	CB-CG	7.44	1.66	1.52
1	A	285	GLU	CD-OE1	7.44	1.33	1.25
1	B	225	VAL	CB-CG2	7.29	1.68	1.52
1	B	77	GLU	CG-CD	7.26	1.62	1.51
1	C	360	ALA	CA-CB	6.99	1.67	1.52
1	C	209	GLU	CG-CD	6.69	1.61	1.51
1	D	344	GLU	CG-CD	6.66	1.61	1.51
1	A	124	CYS	CB-SG	-6.65	1.71	1.82
1	A	285	GLU	CD-OE2	6.53	1.32	1.25
1	B	182	LYS	CD-CE	6.51	1.67	1.51
1	D	285	GLU	CG-CD	6.46	1.61	1.51
1	B	212	PHE	CE1-CZ	6.28	1.49	1.37
1	C	470	TYR	CD1-CE1	6.26	1.48	1.39
1	C	412	PHE	CE2-CZ	6.26	1.49	1.37
1	D	285	GLU	CD-OE1	6.25	1.32	1.25
1	C	502	TYR	CD1-CE1	6.09	1.48	1.39
1	A	132	GLU	CG-CD	6.08	1.61	1.51
1	D	483	LYS	CE-NZ	6.08	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	GLU	CG-CD	6.05	1.61	1.51
1	C	246	GLU	CG-CD	6.05	1.61	1.51
1	D	357	GLU	CG-CD	6.03	1.61	1.51
1	B	171	TRP	CE3-CZ3	6.00	1.48	1.38
1	C	482	GLU	CD-OE2	5.95	1.32	1.25
1	B	360	ALA	CA-CB	5.95	1.65	1.52
1	C	503	LYS	CA-CB	5.95	1.67	1.53
1	B	132	GLU	CG-CD	5.82	1.60	1.51
1	C	419	TRP	CZ3-CH2	5.74	1.49	1.40
1	D	289	TYR	CD1-CE1	5.66	1.47	1.39
1	A	288	GLY	N-CA	5.65	1.54	1.46
1	B	168	TRP	CG-CD1	5.64	1.44	1.36
1	B	391	PHE	CD1-CE1	5.63	1.50	1.39
1	D	97	LYS	CE-NZ	5.63	1.63	1.49
1	A	152	TYR	CG-CD1	5.63	1.46	1.39
1	B	44	TYR	CD1-CE1	5.62	1.47	1.39
1	B	265	GLU	CG-CD	5.59	1.60	1.51
1	A	105	GLU	CG-CD	5.56	1.60	1.51
1	C	257	ASP	CB-CG	5.55	1.63	1.51
1	D	273	SER	CB-OG	5.54	1.49	1.42
1	A	482	GLU	CD-OE2	5.53	1.31	1.25
1	C	216	PHE	CE2-CZ	5.45	1.47	1.37
1	B	288	GLY	N-CA	5.45	1.54	1.46
1	A	97	LYS	CE-NZ	5.44	1.62	1.49
1	A	397	PHE	CD1-CE1	5.44	1.50	1.39
1	C	239	TYR	CD1-CE1	5.43	1.47	1.39
1	B	110	GLU	CB-CG	5.42	1.62	1.52
1	B	119	VAL	CB-CG1	-5.40	1.41	1.52
1	D	482	GLU	CD-OE1	5.39	1.31	1.25
1	D	337	GLU	CG-CD	5.34	1.59	1.51
1	C	97	LYS	CE-NZ	5.33	1.62	1.49
1	B	476	TYR	CD1-CE1	5.30	1.47	1.39
1	C	250	VAL	CB-CG1	5.28	1.64	1.52
1	B	195	ARG	CZ-NH2	5.28	1.40	1.33
1	B	232	GLU	CG-CD	5.27	1.59	1.51
1	B	105	GLU	CG-CD	5.26	1.59	1.51
1	A	131	GLU	CG-CD	5.21	1.59	1.51
1	C	162	GLN	CG-CD	5.20	1.63	1.51
1	C	64	PHE	CE2-CZ	5.15	1.47	1.37
1	B	13	PHE	CG-CD2	-5.15	1.31	1.38
1	C	72	GLY	N-CA	5.14	1.53	1.46
1	D	382	PHE	CE1-CZ	5.12	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	GLU	CD-OE2	-5.10	1.20	1.25
1	D	81	HIS	N-CA	5.10	1.56	1.46
1	B	105	GLU	CD-OE2	5.07	1.31	1.25
1	D	285	GLU	CD-OE2	5.05	1.31	1.25
1	D	344	GLU	CD-OE2	5.03	1.31	1.25

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	D	91	ASP	CB-CG-OD1	11.08	128.27	118.30
1	B	238	ASP	CB-CG-OD1	10.83	128.05	118.30
1	A	83	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	B	74	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	B	181	ASP	CB-CG-OD1	9.30	126.67	118.30
1	A	181	ASP	CB-CG-OD1	8.80	126.22	118.30
1	A	41	ARG	NE-CZ-NH1	-8.73	115.94	120.30
1	C	181	ASP	CB-CG-OD1	7.86	125.37	118.30
1	C	451	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	31	ASP	CB-CG-OD1	7.75	125.27	118.30
1	A	181	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	83	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	C	309	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	D	80	ASP	CB-CG-OD1	7.55	125.10	118.30
1	A	397	PHE	CB-CG-CD2	-7.53	115.53	120.80
1	C	309	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	B	445	PHE	CB-CG-CD2	7.35	125.94	120.80
1	B	238	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	D	91	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	74	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	B	388	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	83	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	C	329	LEU	CB-CG-CD1	-6.66	99.68	111.00
1	D	62	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	D	351	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	80	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	476	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	D	97	LYS	CD-CE-NZ	6.54	126.73	111.70
1	C	44	TYR	CB-CG-CD2	-6.49	117.10	121.00
1	C	181	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	101	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	180	ASP	CB-CG-OD1	6.34	124.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	309	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	19	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	357	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	C	392	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	238	ASP	CB-CG-OD1	6.18	123.86	118.30
1	D	481	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	B	181	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	D	181	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	D	388	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	90	LEU	CB-CG-CD2	5.97	121.14	111.00
1	D	347	LEU	CB-CG-CD1	-5.94	100.90	111.00
1	D	324	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	397	PHE	CB-CG-CD2	-5.92	116.66	120.80
1	C	353	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	238	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	502	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	A	476	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	B	310	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	D	397	PHE	CB-CG-CD1	-5.69	116.81	120.80
1	A	368	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	388	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	238	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	239	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	A	175	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	74	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	257	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	12	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	309	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	390	TYR	CD1-CE1-CZ	-5.49	114.86	119.80
1	C	83	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	16	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	C	165	ASP	CB-CG-OD1	5.44	123.19	118.30
1	C	239	TYR	CB-CG-CD2	-5.39	117.76	121.00
1	D	391	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	91	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	368	ASP	CB-CG-OD1	5.34	123.10	118.30
1	D	369	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	B	44	TYR	CZ-CE2-CD2	-5.30	115.03	119.80
1	A	407	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	44	TYR	CG-CD1-CE1	-5.26	117.09	121.30
1	A	23	LEU	CB-CG-CD1	5.26	119.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	PHE	CB-CG-CD1	-5.26	117.12	120.80
1	D	19	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	491	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	180	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	351	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	390	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	C	481	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	C	143	TYR	N-CA-C	-5.14	97.12	111.00
1	B	80	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	11	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	19	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4052	0	4048	45	0
1	B	4032	0	4021	38	0
1	C	3975	0	3963	44	0
1	D	4032	0	4026	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	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
4	D	1	0	0	0	0
5	A	36	0	28	4	0
5	B	36	0	28	4	0
5	C	36	0	27	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	36	0	28	3	0
6	A	437	0	0	23	1
6	B	358	0	0	12	1
6	C	275	0	0	6	0
6	D	377	0	0	13	0
All	All	17693	0	16169	178	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (178) 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:430:ASP:CG	6:A:701:HOH:O	1.69	1.31
1:B:28[B]:GLU:OE2	6:B:701:HOH:O	1.56	1.22
1:D:368:ASP:CG	6:D:701:HOH:O	1.77	1.22
5:C:603:4LU:H14	5:C:603:4LU:H5	1.34	1.08
5:A:604:4LU:H5	5:A:604:4LU:H14	1.34	1.04
5:D:603:4LU:H14	5:D:603:4LU:H5	1.41	0.99
1:A:483:LYS:HE3	6:A:957:HOH:O	1.65	0.97
5:A:604:4LU:H14	5:A:604:4LU:C13	1.97	0.94
5:C:603:4LU:H14	5:C:603:4LU:C13	1.98	0.93
5:D:603:4LU:H14	5:D:603:4LU:C13	1.98	0.92
1:D:368:ASP:OD1	6:D:701:HOH:O	1.77	0.91
1:B:77:GLU:HG3	6:B:943:HOH:O	1.74	0.87
1:D:166:LYS:NZ	6:D:704:HOH:O	2.07	0.85
1:D:344:GLU:OE2	6:D:702:HOH:O	1.95	0.84
1:C:344:GLU:OE2	6:C:701:HOH:O	1.96	0.82
5:B:604:4LU:H14	5:B:604:4LU:H5	1.59	0.82
1:D:428:VAL:H	1:D:431:GLN:HE21	1.28	0.81
1:A:61:LYS:HD3	6:A:950:HOH:O	1.80	0.81
1:A:61:LYS:HD2	6:A:959:HOH:O	1.78	0.81
1:A:430:ASP:OD1	6:A:701:HOH:O	1.83	0.81
1:D:482:GLU:OE2	6:D:703:HOH:O	1.99	0.80
1:B:130:SER:HB2	6:B:1007:HOH:O	1.81	0.80
1:B:322:CYS:H	1:B:359:GLN:HE22	1.27	0.79
1:B:127:HIS:HE1	1:B:310:ASP:OD1	1.64	0.79
1:B:428:VAL:H	1:B:431:GLN:HE21	1.28	0.78
1:B:1:MET:HG2	6:B:837:HOH:O	1.84	0.78
1:A:61:LYS:CG	6:A:1067:HOH:O	2.31	0.76
1:A:61:LYS:CD	6:A:959:HOH:O	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:HG3	6:A:1057:HOH:O	1.86	0.76
5:B:604:4LU:H14	5:B:604:4LU:C13	2.16	0.74
1:C:81:HIS:HE1	1:C:356:TYR:OH	1.70	0.73
1:B:81:HIS:HE1	1:B:356:TYR:OH	1.71	0.73
1:C:428:VAL:H	1:C:431:GLN:HE21	1.35	0.73
1:A:428:VAL:H	1:A:431:GLN:HE21	1.36	0.72
1:A:81:HIS:HE1	1:A:356:TYR:OH	1.71	0.71
1:D:294:GLN:HE22	1:D:448:GLN:HE22	1.38	0.71
1:A:145:HIS:HE1	1:A:319:PRO:O	1.74	0.70
1:A:5:ASN:OD1	6:A:702:HOH:O	2.09	0.69
1:A:322:CYS:H	1:A:359:GLN:HE22	1.39	0.69
1:D:81:HIS:HE1	1:D:356:TYR:OH	1.75	0.69
1:D:322:CYS:H	1:D:359:GLN:HE22	1.40	0.68
1:B:77:GLU:CG	6:B:943:HOH:O	2.37	0.68
1:B:145:HIS:HE1	1:B:319:PRO:O	1.77	0.67
1:A:61:LYS:HG3	6:A:1067:HOH:O	1.93	0.67
1:D:428:VAL:H	1:D:431:GLN:NE2	1.92	0.67
1:B:294:GLN:HE22	1:B:448:GLN:HE22	1.42	0.67
1:B:428:VAL:H	1:B:431:GLN:NE2	1.92	0.67
1:D:127:HIS:HE1	1:D:310:ASP:OD1	1.78	0.67
1:D:145:HIS:HD2	1:D:148:ASP:OD2	1.78	0.66
1:A:127:HIS:HE1	1:A:310:ASP:OD1	1.77	0.66
1:A:436[B]:ASP:O	6:A:703:HOH:O	2.15	0.64
1:C:453:LYS:HA	1:C:453:LYS:HE3	1.80	0.64
1:B:441:PRO:HB3	1:B:455:MET:HE3	1.80	0.63
1:C:428:VAL:H	1:C:431:GLN:NE2	1.96	0.63
1:A:455:MET:HB3	6:A:855:HOH:O	1.98	0.63
1:A:392[B]:ARG:HB2	6:A:729:HOH:O	1.97	0.63
1:A:430:ASP:CB	6:A:701:HOH:O	2.32	0.62
1:C:145:HIS:HD2	1:C:148:ASP:OD2	1.83	0.62
1:D:368:ASP:CB	6:D:701:HOH:O	2.36	0.61
1:C:322:CYS:H	1:C:359:GLN:HE22	1.47	0.60
1:B:137[B]:GLN:HA	1:B:137[B]:GLN:HE21	1.68	0.59
1:D:61:LYS:HE3	6:D:706:HOH:O	2.02	0.59
1:D:71:ALA:HB3	1:D:325:GLU:HG3	1.85	0.59
5:B:604:4LU:H6	5:B:604:4LU:O4	2.01	0.59
1:A:145:HIS:HD2	1:A:148:ASP:OD2	1.86	0.58
1:B:145:HIS:HD2	1:B:148:ASP:OD2	1.86	0.58
1:C:467:ARG:HH21	1:C:467:ARG:HG3	1.68	0.58
1:A:287:HIS:HD2	6:A:1059:HOH:O	1.87	0.58
1:A:487:LYS:HE2	6:A:1084:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ASP:OD1	1:D:81:HIS:HD2	1.87	0.57
1:A:428:VAL:H	1:A:431:GLN:NE2	2.01	0.57
1:C:294:GLN:HE22	1:C:448:GLN:HE22	1.51	0.57
1:D:145:HIS:HE1	1:D:319:PRO:O	1.88	0.57
1:B:71:ALA:HB3	1:B:325:GLU:HG3	1.87	0.56
1:A:80:ASP:OD1	1:A:81:HIS:HD2	1.88	0.56
1:C:224:LEU:C	1:C:224:LEU:HD23	2.27	0.55
1:B:69:CYS:N	1:B:70:PRO:CD	2.70	0.55
1:D:114:PRO:HG3	1:D:237:SER:HB2	1.89	0.54
1:D:287:HIS:HE1	6:D:856:HOH:O	1.91	0.54
5:D:603:4LU:O4	5:D:603:4LU:H6	2.07	0.54
1:D:287:HIS:HD2	6:D:1022:HOH:O	1.90	0.54
1:C:80:ASP:OD1	1:C:81:HIS:HD2	1.91	0.54
1:C:283:PHE:O	1:C:285[B]:GLU:HG3	2.07	0.53
1:C:84:ILE:H	1:C:84:ILE:HD12	1.73	0.53
1:C:467:ARG:NH2	1:C:471:GLU:OE2	2.41	0.53
1:A:109:LYS:HE2	6:B:1007:HOH:O	2.08	0.52
1:B:287:HIS:HE1	6:B:876:HOH:O	1.92	0.52
1:B:322:CYS:N	1:B:359:GLN:HE22	2.02	0.52
1:A:287:HIS:HE1	6:A:782:HOH:O	1.93	0.51
1:C:4:LEU:CD1	1:C:16[B]:VAL:HG12	2.41	0.50
1:C:145:HIS:HE1	1:C:319:PRO:O	1.92	0.50
1:C:114:PRO:HG3	1:C:237:SER:HB2	1.94	0.50
1:A:28:GLU:OE2	6:A:704:HOH:O	2.19	0.50
1:C:287:HIS:HE1	6:C:788:HOH:O	1.96	0.49
1:C:287:HIS:HD2	6:C:836:HOH:O	1.96	0.49
1:D:287:HIS:CD2	6:D:1022:HOH:O	2.65	0.49
1:B:287:HIS:HD2	6:B:1009:HOH:O	1.95	0.48
1:C:287:HIS:CD2	6:C:836:HOH:O	2.65	0.48
1:A:344:GLU:CG	6:A:1057:HOH:O	2.54	0.48
5:A:604:4LU:O4	5:A:604:4LU:H6	2.13	0.48
1:D:105:GLU:CD	6:D:707:HOH:O	2.52	0.48
1:D:376:LYS:HE3	6:D:830:HOH:O	2.12	0.48
1:A:208[A]:ASN:ND2	1:A:273:SER:OG	2.46	0.48
1:C:306[B]:MET:HB2	1:C:306[B]:MET:HE2	1.68	0.48
1:C:12:ASP:O	1:C:16[B]:VAL:HG13	2.14	0.48
1:A:173:ILE:HD12	1:A:227[B]:SER:OG	2.14	0.48
1:C:467:ARG:HG3	1:C:467:ARG:NH2	2.29	0.48
1:D:441:PRO:HA	1:D:455[C]:MET:HE1	1.95	0.48
5:C:603:4LU:H6	5:C:603:4LU:O4	2.14	0.47
5:B:604:4LU:H22	5:B:604:4LU:H7	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:HIS:HE1	1:C:310:ASP:OD1	1.97	0.47
1:A:294:GLN:HE22	1:A:448:GLN:HE22	1.62	0.47
1:A:355:PRO:HD3	1:A:364:ILE:HG12	1.97	0.47
1:B:287:HIS:CD2	6:B:1009:HOH:O	2.67	0.47
1:C:491:ASP:O	1:C:495:GLU:HG3	2.15	0.47
1:A:188:VAL:HG12	1:A:195[A]:ARG:HD3	1.98	0.46
1:A:431:GLN:HB3	1:A:460[B]:CYS:SG	2.56	0.46
1:D:69:CYS:N	1:D:70:PRO:CD	2.79	0.46
1:C:4:LEU:HD13	1:C:16[B]:VAL:HG12	1.97	0.46
1:B:287:HIS:CD2	1:B:444:PRO:HD3	2.50	0.46
1:B:24:ILE:HG12	1:B:49:PRO:HB2	1.97	0.45
1:B:84:ILE:H	1:B:84:ILE:HD12	1.80	0.45
1:D:127:HIS:CE1	1:D:310:ASP:OD1	2.64	0.45
1:B:201:TRP:HB2	1:B:210:ILE:HG12	1.98	0.45
1:A:477:ILE:HB	1:D:290:VAL:HB	1.98	0.45
1:C:453:LYS:HA	1:C:453:LYS:CE	2.44	0.45
1:A:387:GLY:HA3	1:A:434:PHE:CZ	2.52	0.45
1:D:355:PRO:HD3	1:D:364:ILE:HG12	1.99	0.45
1:A:69:CYS:N	1:A:70:PRO:CD	2.79	0.45
1:D:145:HIS:CD2	1:D:148:ASP:OD2	2.65	0.45
1:A:71:ALA:HB3	1:A:325:GLU:HG3	1.98	0.44
1:B:208[A]:ASN:ND2	1:B:273:SER:OG	2.42	0.44
1:C:322:CYS:HA	1:C:323:THR:HA	1.82	0.44
1:A:61:LYS:HG2	6:A:1067:HOH:O	2.09	0.43
1:C:326:THR:O	1:C:330:ILE:HB	2.18	0.43
1:C:80:ASP:OD1	6:C:702:HOH:O	2.21	0.43
1:A:132:GLU:HB3	6:A:894:HOH:O	2.19	0.43
1:B:455:MET:HE3	6:B:765:HOH:O	2.19	0.43
1:C:387:GLY:HA3	1:C:434:PHE:CZ	2.53	0.43
1:D:173:ILE:HD12	1:D:227[B]:SER:OG	2.19	0.43
1:D:454:THR:O	1:D:455[A]:MET:HB2	2.19	0.43
1:A:287:HIS:CD2	6:A:1059:HOH:O	2.68	0.42
1:B:134:ILE:CD1	1:B:306[A]:MET:HB3	2.49	0.42
1:C:270:GLY:HA3	1:C:302:THR:O	2.19	0.42
1:D:455[C]:MET:HE3	1:D:455[C]:MET:HA	2.00	0.42
1:C:251:VAL:CG2	6:C:944:HOH:O	2.67	0.42
5:A:604:4LU:C7M	5:A:604:4LU:C13	2.78	0.42
1:C:431:GLN:HB3	1:C:460[B]:CYS:SG	2.59	0.42
1:B:201:TRP:CB	1:B:210:ILE:HG12	2.50	0.42
1:B:28[B]:GLU:CD	1:B:28[B]:GLU:H	2.22	0.42
1:D:275:THR:HG21	6:D:887:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PRO:HG3	1:A:237:SER:HB2	2.01	0.42
1:B:127:HIS:CE1	1:B:310:ASP:OD1	2.56	0.42
1:A:218:VAL:HB	1:A:219:PRO:HD2	2.02	0.42
1:D:224:LEU:C	1:D:224:LEU:HD23	2.41	0.42
1:B:455:MET:HG3	6:B:919:HOH:O	2.19	0.41
1:C:134:ILE:HD13	1:C:306[B]:MET:HE3	2.02	0.41
1:A:145:HIS:CD2	1:A:148:ASP:OD2	2.71	0.41
1:B:21:ASP:HA	6:B:841:HOH:O	2.20	0.41
1:D:387:GLY:HA3	1:D:434:PHE:CZ	2.56	0.41
1:C:13:PHE:O	1:C:17:LEU:HG	2.21	0.41
1:B:497:TRP:O	1:B:500[B]:TYR:O	2.39	0.41
1:C:218:VAL:HB	1:C:219:PRO:HD2	2.03	0.41
1:B:114:PRO:HG3	1:B:237:SER:HB2	2.01	0.41
1:B:69:CYS:N	1:B:70:PRO:HD2	2.36	0.41
1:C:230:ILE:HB	1:C:231:PRO:CD	2.51	0.41
1:C:287:HIS:CD2	1:C:444:PRO:HD3	2.56	0.41
1:C:46:SER:HB2	1:C:48:LEU:HG	2.02	0.41
1:C:173:ILE:HD12	5:C:603:4LU:H19	2.02	0.41
1:C:453:LYS:CE	1:C:453:LYS:CA	2.99	0.41
1:C:306[A]:MET:HG2	1:C:307:SER:N	2.35	0.40
1:B:80:ASP:OD1	1:B:81:HIS:HD2	2.04	0.40
1:D:294:GLN:HE22	1:D:448:GLN:NE2	2.13	0.40
1:C:209:GLU:O	1:C:209:GLU:HG3	2.21	0.40
1:A:115:ILE:HD12	6:A:1045:HOH:O	2.19	0.40
1:B:500[B]:TYR:O	1:B:502:TYR:N	2.54	0.40
1:D:322:CYS:N	1:D:359:GLN:HE22	2.15	0.40
1:D:24:ILE:HG12	1:D:49:PRO:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:878:HOH:O	6:B:978:HOH:O[2_646]	2.15	0.05

## 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	515/503 (102%)	506 (98%)	9 (2%)	0	100	100
1	B	512/503 (102%)	497 (97%)	14 (3%)	1 (0%)	47	28
1	C	508/503 (101%)	495 (97%)	13 (3%)	0	100	100
1	D	513/503 (102%)	503 (98%)	10 (2%)	0	100	100
All	All	2048/2012 (102%)	2001 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ARG

### 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	451/438 (103%)	444 (98%)	7 (2%)	62	41
1	B	447/438 (102%)	439 (98%)	8 (2%)	59	36
1	C	441/438 (101%)	433 (98%)	8 (2%)	59	36
1	D	449/438 (102%)	443 (99%)	6 (1%)	69	50
All	All	1788/1752 (102%)	1759 (98%)	29 (2%)	62	41

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	LYS
1	A	78	LYS
1	A	132	GLU
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	181	ASP
1	A	220	PRO
1	B	61	LYS
1	B	64	PHE
1	B	77	GLU
1	B	181	ASP
1	B	306[A]	MET
1	B	306[B]	MET
1	B	370	LYS
1	B	460	CYS
1	C	64	PHE
1	C	108	GLU
1	C	137	GLN
1	C	154	GLN
1	C	181	ASP
1	C	220	PRO
1	C	279	LEU
1	C	453	LYS
1	D	61	LYS
1	D	64	PHE
1	D	137	GLN
1	D	154	GLN
1	D	181	ASP
1	D	498	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	127	HIS
1	A	145	HIS
1	A	287	HIS
1	A	294	GLN
1	A	296	HIS
1	A	359	GLN
1	A	431	GLN
1	B	81	HIS
1	B	127	HIS
1	B	145	HIS
1	B	287	HIS
1	B	359	GLN
1	B	431	GLN

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Mol	Chain	Res	Type
1	B	448	GLN
1	C	81	HIS
1	C	127	HIS
1	C	137	GLN
1	C	145	HIS
1	C	287	HIS
1	C	359	GLN
1	C	431	GLN
1	C	448	GLN
1	D	81	HIS
1	D	127	HIS
1	D	145	HIS
1	D	287	HIS
1	D	359	GLN
1	D	431	GLN
1	D	448	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 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
5	4LU	C	603	3,4	32,39,39	3.16	10 (31%)	41,62,62	2.65	17 (41%)
5	4LU	D	603	3,4	32,39,39	1.85	7 (21%)	41,62,62	2.25	9 (21%)
5	4LU	B	604	3,4	32,39,39	2.38	9 (28%)	41,62,62	2.99	18 (43%)
5	4LU	A	604	3,4	32,39,39	1.99	11 (34%)	41,62,62	2.78	15 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	4LU	C	603	3,4	-	4/18/30/30	0/3/4/4
5	4LU	D	603	3,4	-	0/18/30/30	0/3/4/4
5	4LU	B	604	3,4	-	2/18/30/30	0/3/4/4
5	4LU	A	604	3,4	-	1/18/30/30	0/3/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	603	4LU	C4-N3	8.82	1.48	1.33
5	C	603	4LU	C10-N1	8.04	1.43	1.33
5	B	604	4LU	C4-N3	7.63	1.46	1.33
5	C	603	4LU	C2'-C3'	-6.75	1.40	1.53
5	C	603	4LU	C5'-C4'	6.44	1.60	1.51
5	D	603	4LU	C4-N3	5.89	1.43	1.33
5	B	604	4LU	C10-N1	5.49	1.40	1.33
5	C	603	4LU	C4'-C3'	-5.32	1.43	1.53
5	A	604	4LU	C10-N1	4.76	1.39	1.33
5	A	604	4LU	C4-N3	4.35	1.40	1.33
5	B	604	4LU	C3-C5	-4.12	1.48	1.54
5	B	604	4LU	C9A-N10	4.09	1.44	1.38
5	A	604	4LU	C2'-C3'	-4.00	1.45	1.53
5	D	603	4LU	C2'-C3'	-3.87	1.46	1.53
5	D	603	4LU	C10-N1	3.73	1.38	1.33
5	D	603	4LU	C3-C5	-3.58	1.49	1.54
5	C	603	4LU	O3'-C3'	3.40	1.51	1.43
5	A	604	4LU	C2-N3	-3.23	1.31	1.38
5	A	604	4LU	C7M-C7	3.11	1.58	1.51
5	B	604	4LU	C4-C4A	-3.11	1.36	1.41
5	C	603	4LU	C2-N3	-3.08	1.32	1.38
5	C	603	4LU	C3-C5	-2.98	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	4LU	C5-C6	-2.92	1.42	1.54
5	A	604	4LU	C9A-N10	2.86	1.42	1.38
5	B	604	4LU	C5'-C4'	2.77	1.55	1.51
5	A	604	4LU	C3-C5	-2.64	1.50	1.54
5	A	604	4LU	C5'-C4'	2.55	1.55	1.51
5	C	603	4LU	C5-C6	-2.46	1.44	1.54
5	B	604	4LU	C2-N3	-2.45	1.33	1.38
5	A	604	4LU	C5-C6	-2.38	1.44	1.54
5	D	603	4LU	C8M-C8	-2.31	1.46	1.51
5	D	603	4LU	C9-C8	2.21	1.43	1.37
5	A	604	4LU	C13-C5	2.14	1.59	1.53
5	D	603	4LU	C5'-C4'	2.08	1.54	1.51
5	A	604	4LU	C1'-N10	-2.06	1.46	1.48
5	C	603	4LU	C9-C8	2.06	1.42	1.37
5	B	604	4LU	C9-C8	2.06	1.42	1.37

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	603	4LU	C13-C5-C6	8.60	120.14	111.72
5	B	604	4LU	C13-C5-C6	8.05	119.60	111.72
5	A	604	4LU	C4-N3-C2	7.81	121.74	115.14
5	B	604	4LU	C1'-N10-C9A	6.50	123.41	118.29
5	B	604	4LU	C9A-N10-C10	-6.31	113.65	121.91
5	C	603	4LU	C13-C5-C6	6.15	117.74	111.72
5	D	603	4LU	C4-C4A-C10	-5.97	116.00	119.95
5	A	604	4LU	C9-C8-C7	5.84	125.79	119.87
5	A	604	4LU	C1'-N10-C10	5.79	123.59	118.41
5	A	604	4LU	C4-C4A-C10	-5.71	116.17	119.95
5	C	603	4LU	C5A-C9A-N10	-5.70	115.86	120.43
5	C	603	4LU	C4-N3-C2	5.46	119.75	115.14
5	B	604	4LU	C12-C5-C13	-5.14	97.14	108.67
5	A	604	4LU	C5'-C4'-C3'	-5.06	102.42	112.20
5	B	604	4LU	C4-N3-C2	5.05	119.41	115.14
5	C	603	4LU	C4-C4A-C10	-4.80	116.77	119.95
5	B	604	4LU	C7M-C7-C8	-4.74	110.98	119.71
5	D	603	4LU	C4-N3-C2	4.73	119.13	115.14
5	A	604	4LU	C13-C5-C6	4.58	116.20	111.72
5	A	604	4LU	C7-C6-C5A	-4.50	114.58	119.06
5	C	603	4LU	C7-C6-C5A	-4.39	114.69	119.06
5	B	604	4LU	C8-C7-C6	4.30	123.22	119.43
5	C	603	4LU	C5'-C4'-C3'	-4.19	104.12	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604	4LU	C1'-N10-C10	4.11	122.09	118.41
5	A	604	4LU	O2'-C2'-C3'	3.91	118.61	109.10
5	B	604	4LU	C4A-C10-N10	3.62	124.02	120.30
5	C	603	4LU	C4'-C3'-C2'	3.60	120.84	113.36
5	C	603	4LU	O4'-C4'-C3'	3.59	117.82	109.10
5	C	603	4LU	O3'-C3'-C2'	3.40	117.03	108.81
5	C	603	4LU	P-O5'-C5'	3.17	127.02	118.30
5	A	604	4LU	C9A-N10-C10	-3.11	117.84	121.91
5	A	604	4LU	C8M-C8-C9	-3.04	113.07	120.34
5	B	604	4LU	C13-C5-C3	-3.04	104.33	109.60
5	D	603	4LU	O4'-C4'-C5'	-3.03	103.10	109.92
5	B	604	4LU	C7-C6-C5A	-3.02	116.06	119.06
5	A	604	4LU	C12-C5-C3	3.00	114.80	109.60
5	D	603	4LU	C5'-C4'-C3'	-2.92	106.57	112.20
5	D	603	4LU	C1'-N10-C9A	2.87	120.55	118.29
5	C	603	4LU	C12-C5-C6	-2.86	108.92	111.72
5	B	604	4LU	C8M-C8-C7	2.86	125.62	121.17
5	B	604	4LU	C4-C4A-C10	-2.84	118.07	119.95
5	A	604	4LU	C12-C5-C13	-2.81	102.36	108.67
5	C	603	4LU	C9-C8-C7	2.81	122.72	119.87
5	B	604	4LU	C3-C5-C6	2.78	113.74	107.38
5	A	604	4LU	O3'-C3'-C4'	2.72	115.39	108.81
5	D	603	4LU	C12-C5-C13	-2.65	102.72	108.67
5	C	603	4LU	O2'-C2'-C3'	2.63	115.49	109.10
5	B	604	4LU	C8M-C8-C9	-2.51	114.34	120.34
5	B	604	4LU	C5'-C4'-C3'	-2.38	107.61	112.20
5	B	604	4LU	O2'-C2'-C3'	-2.35	103.38	109.10
5	C	603	4LU	O1P-P-O3P	2.32	116.50	107.64
5	C	603	4LU	C9A-N10-C10	-2.30	118.90	121.91
5	B	604	4LU	O3'-C3'-C2'	-2.28	103.30	108.81
5	D	603	4LU	O2'-C2'-C1'	-2.20	104.30	109.59
5	A	604	4LU	O5'-C5'-C4'	-2.18	103.53	109.36
5	D	603	4LU	C9A-N10-C10	-2.17	119.06	121.91
5	A	604	4LU	O3'-C3'-C2'	2.16	114.04	108.81
5	C	603	4LU	C1'-N10-C9A	2.08	119.93	118.29
5	C	603	4LU	C1'-N10-C10	2.03	120.23	118.41

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	603	4LU	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
5	C	603	4LU	O3'-C3'-C4'-O4'
5	B	604	4LU	C2'-C3'-C4'-C5'
5	C	603	4LU	C5'-O5'-P-O2P
5	C	603	4LU	C4'-C5'-O5'-P
5	B	604	4LU	C4'-C5'-O5'-P
5	A	604	4LU	C4'-C5'-O5'-P

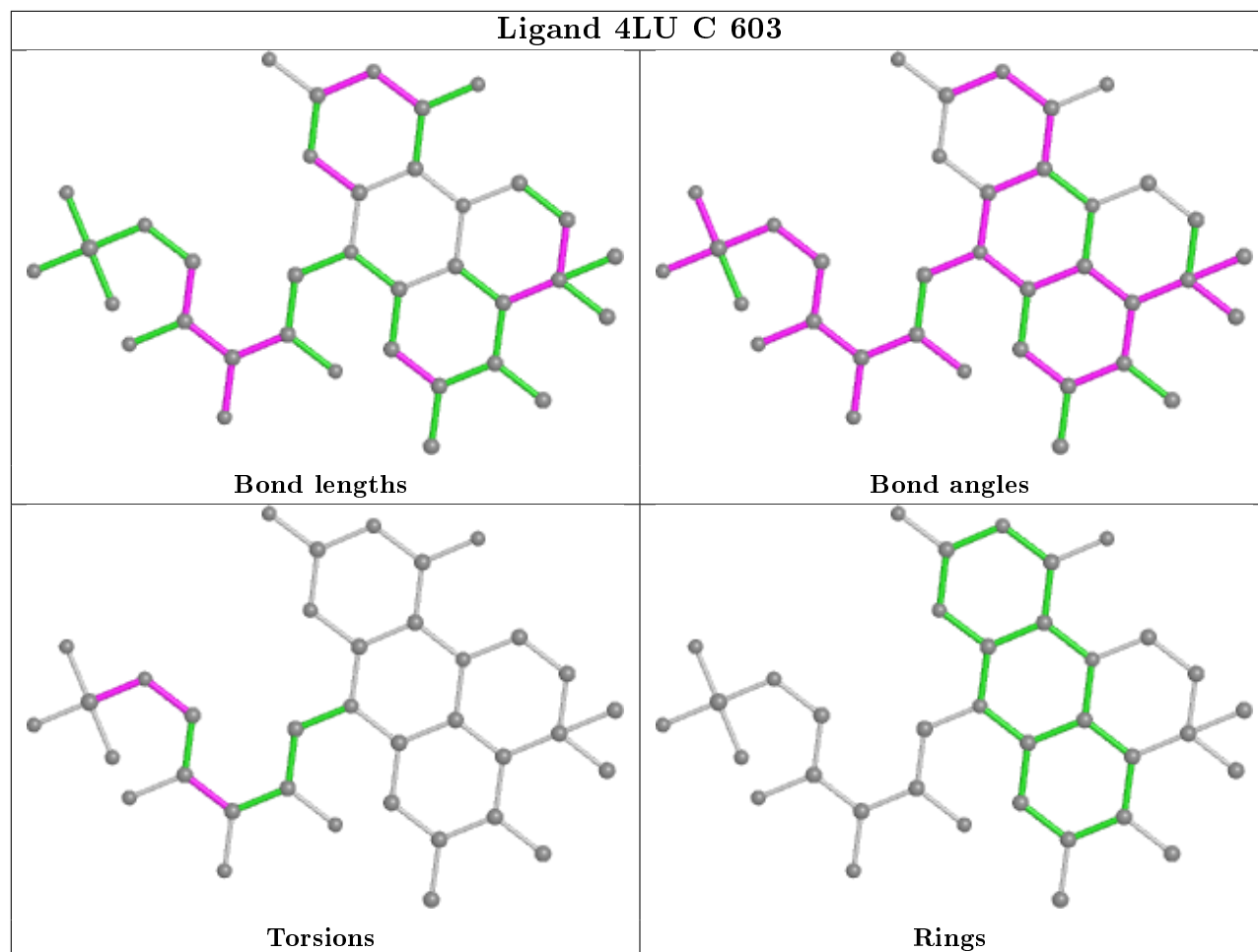
There are no ring outliers.

4 monomers are involved in 15 short contacts:

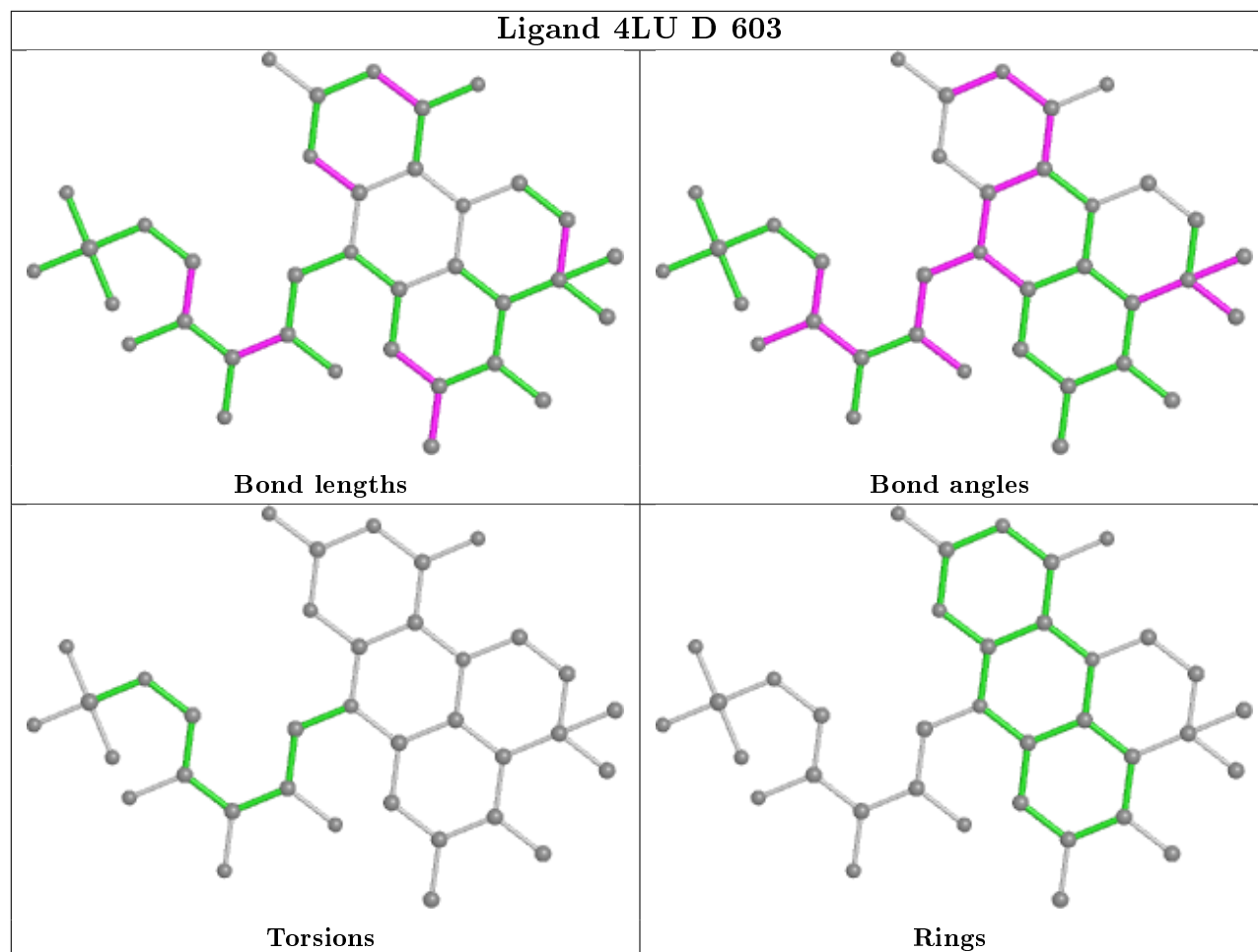
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	603	4LU	4	0
5	D	603	4LU	3	0
5	B	604	4LU	4	0
5	A	604	4LU	4	0

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

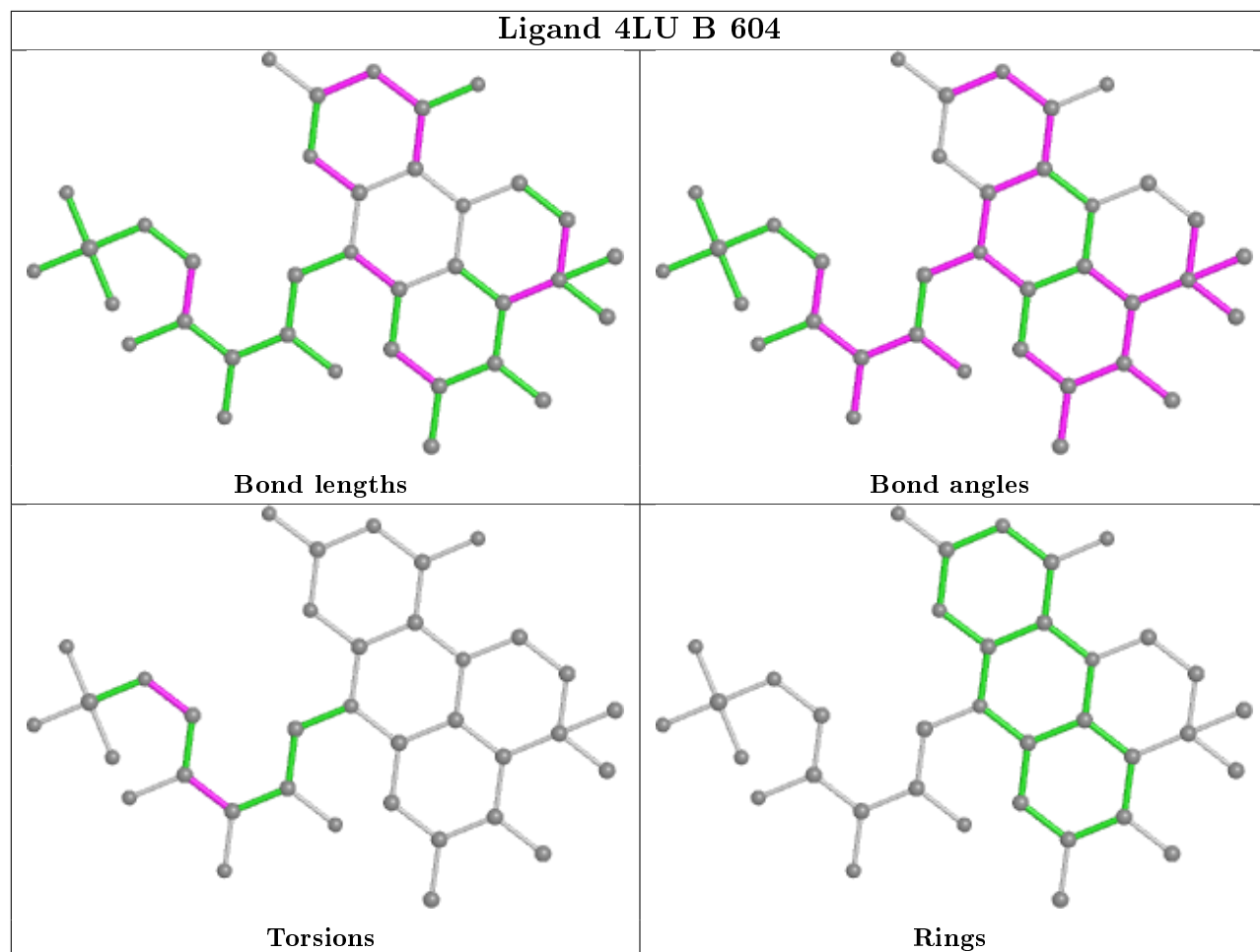
## Ligand 4LU C 603

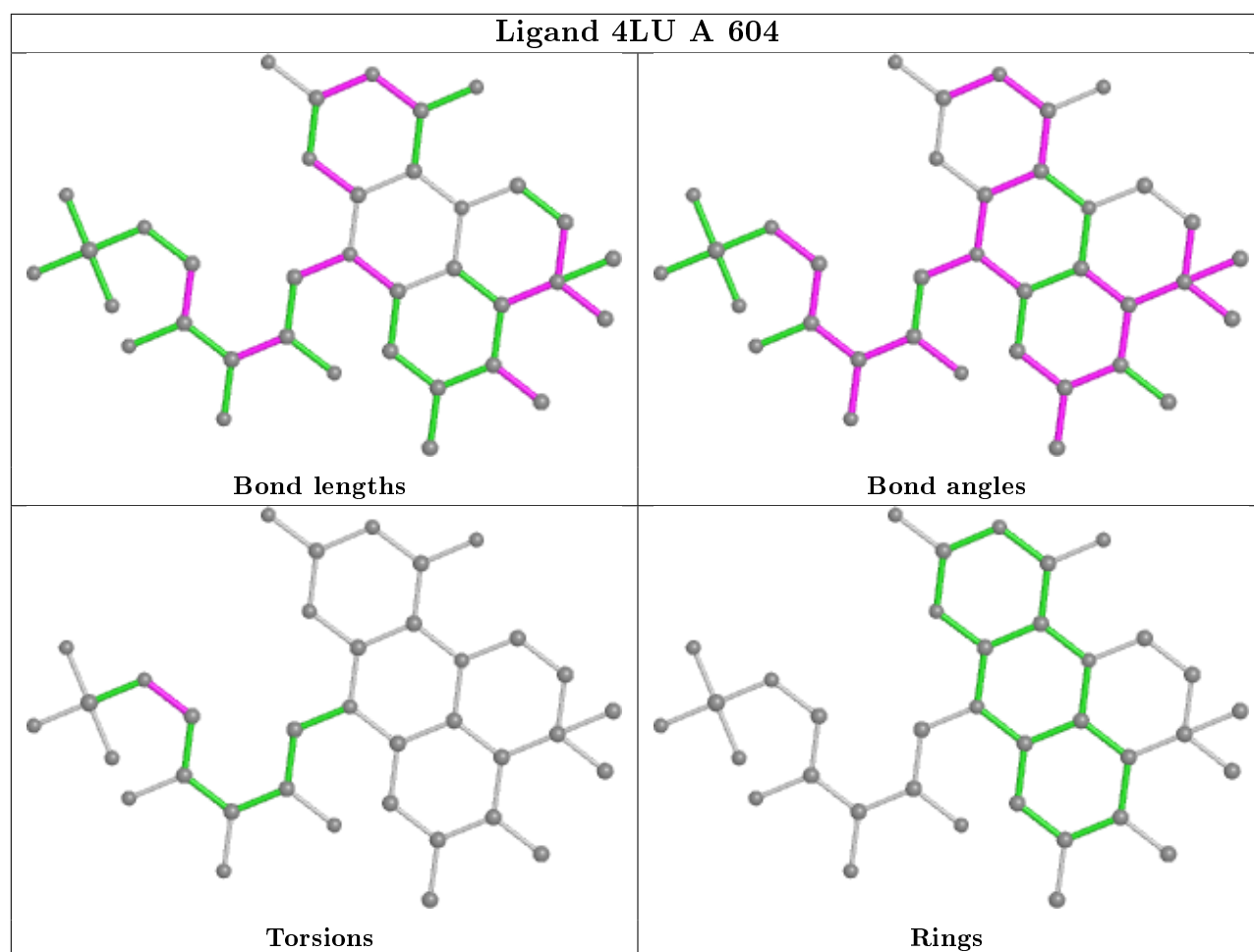


## Ligand 4LU D 603



## Ligand 4LU B 604





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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	503/503 (100%)	-0.45	3 (0%) 89 90	13, 20, 33, 46	0
1	B	503/503 (100%)	-0.48	2 (0%) 92 93	14, 22, 38, 62	0
1	C	501/503 (99%)	-0.37	2 (0%) 92 93	17, 26, 40, 57	0
1	D	503/503 (100%)	-0.38	3 (0%) 89 90	15, 22, 36, 66	0
All	All	2010/2012 (99%)	-0.42	10 (0%) 91 92	13, 22, 38, 66	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	6.5
1	B	1	MET	4.4
1	C	3	LYS	3.4
1	D	2	ARG	3.1
1	C	58	GLY	2.7
1	B	498	LYS	2.5
1	A	295	GLY	2.4
1	A	61	LYS	2.3
1	A	132	GLU	2.2
1	D	132	GLU	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 carbohydrates in this entry.

## 6.4 Ligands

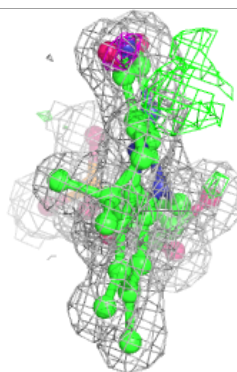
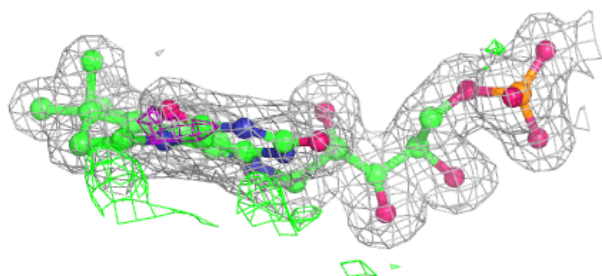
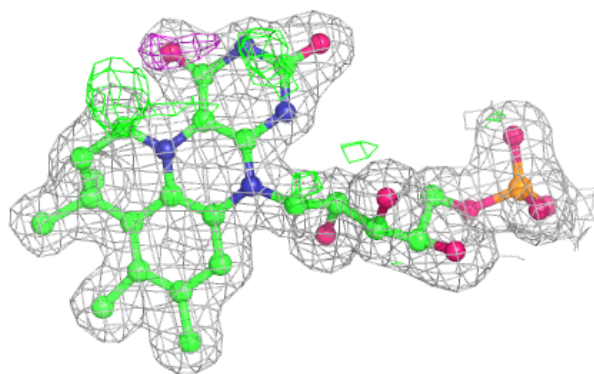
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	C	604	1/1	0.93	0.08	38,38,38,38	0
2	NA	A	601	1/1	0.94	0.05	27,27,27,27	0
2	NA	B	601	1/1	0.97	0.05	22,22,22,22	0
5	4LU	B	604	36/36	0.97	0.07	13,17,24,26	0
5	4LU	A	604	36/36	0.98	0.07	13,15,24,28	0
5	4LU	D	603	36/36	0.98	0.07	15,18,24,27	0
3	K	C	602	1/1	0.98	0.08	21,21,21,21	0
5	4LU	C	603	36/36	0.98	0.08	17,21,28,30	0
4	MN	C	601	1/1	0.98	0.06	21,21,21,21	1
4	MN	A	603	1/1	1.00	0.07	16,16,16,16	1
3	K	B	602	1/1	1.00	0.07	16,16,16,16	0
4	MN	B	603	1/1	1.00	0.05	17,17,17,17	1
3	K	A	602	1/1	1.00	0.07	15,15,15,15	0
4	MN	D	601	1/1	1.00	0.05	20,20,20,20	1
3	K	D	602	1/1	1.00	0.08	18,18,18,18	0

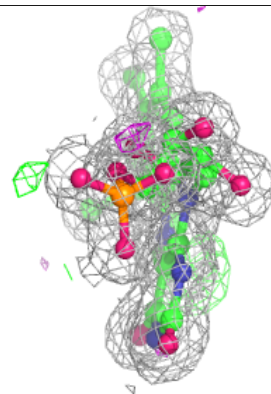
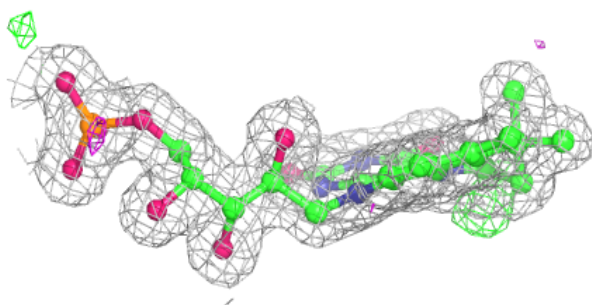
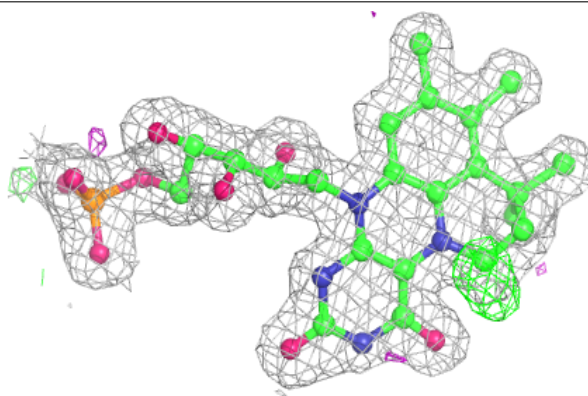
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 4LU B 604:**

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

**Electron density around 4LU A 604:**

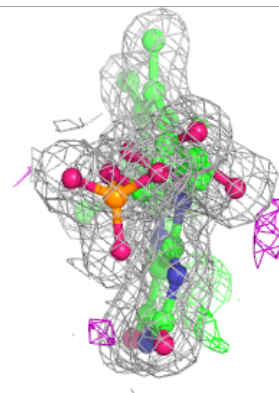
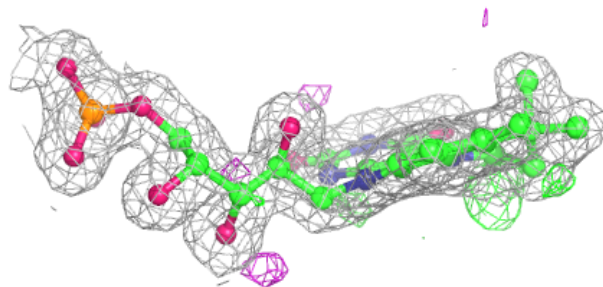
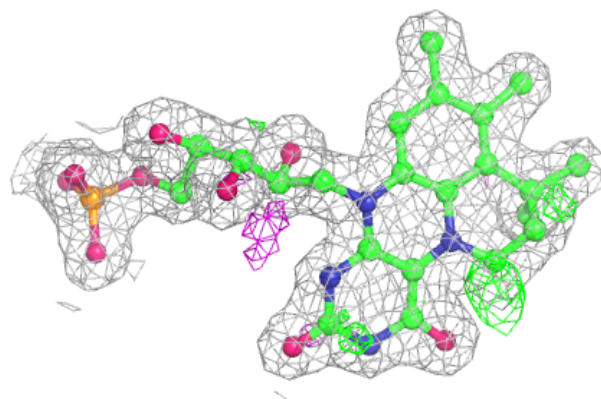
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



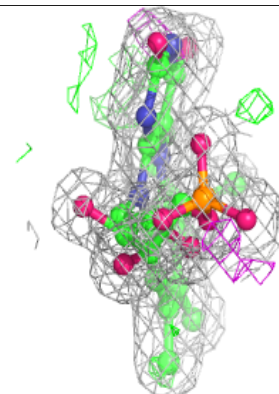
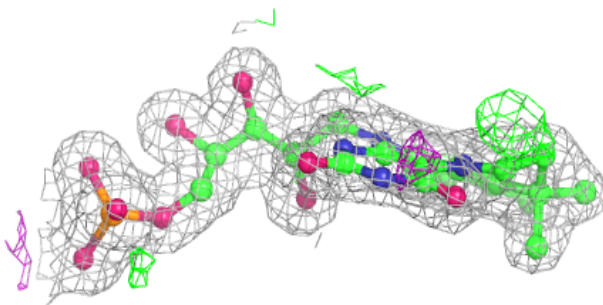
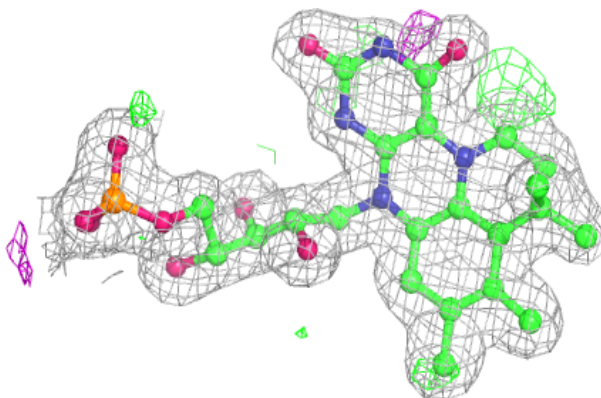


**Electron density around 4LU D 603:**

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

**Electron density around 4LU C 603:**

$2mF_o-DF_c$  (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.