



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:33 PM UTC

PDB ID : 4ZAC / pdb_00004zac
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

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

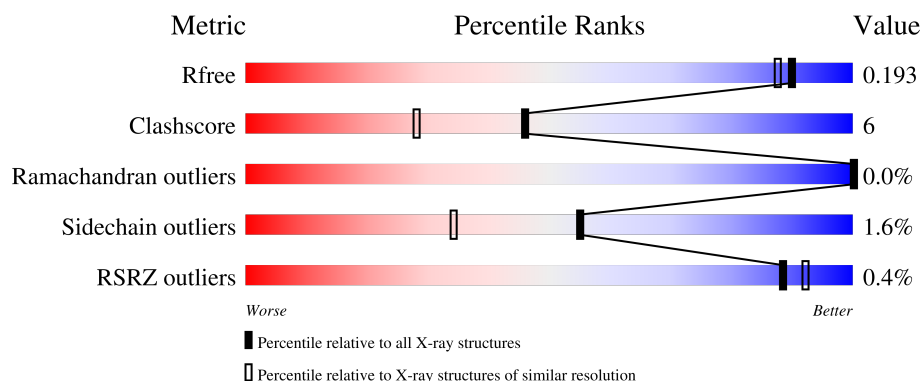
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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 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	503	
1	B	503	
1	C	503	
1	D	503	

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 (CCD ID: NA) (formula: Na).

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

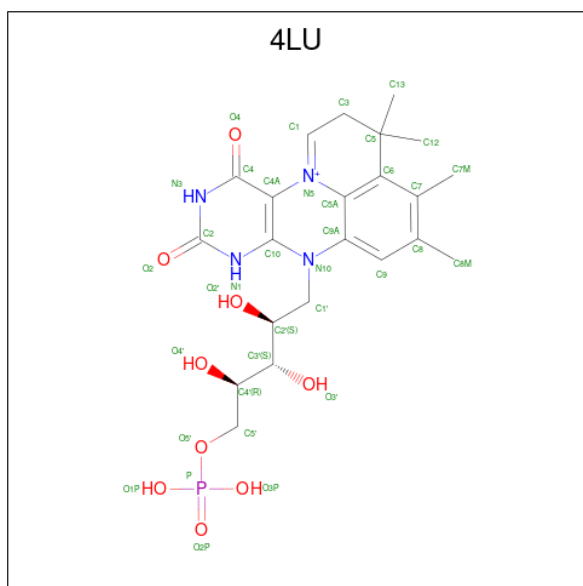
- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	D	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 (CCD ID: 4LU) (formula: $C_{22}H_{30}N_4O_9P$).



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

- Molecule 6 is water.

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

Continued on next page...

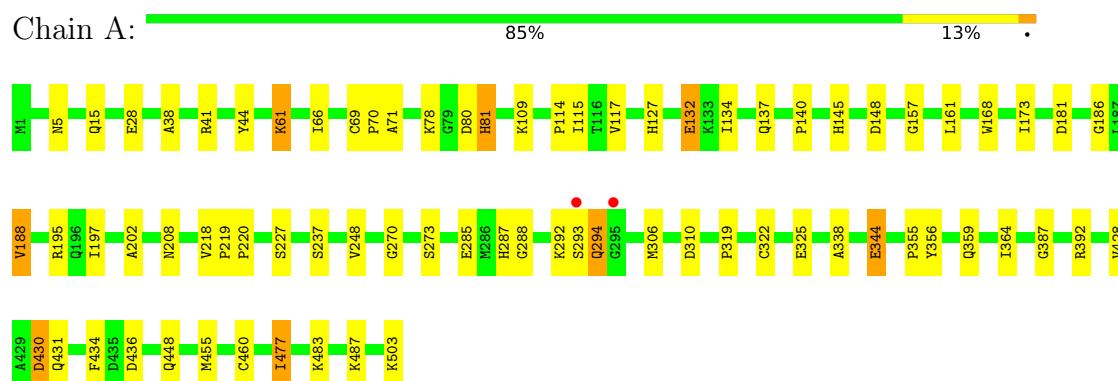
Continued from previous page...

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

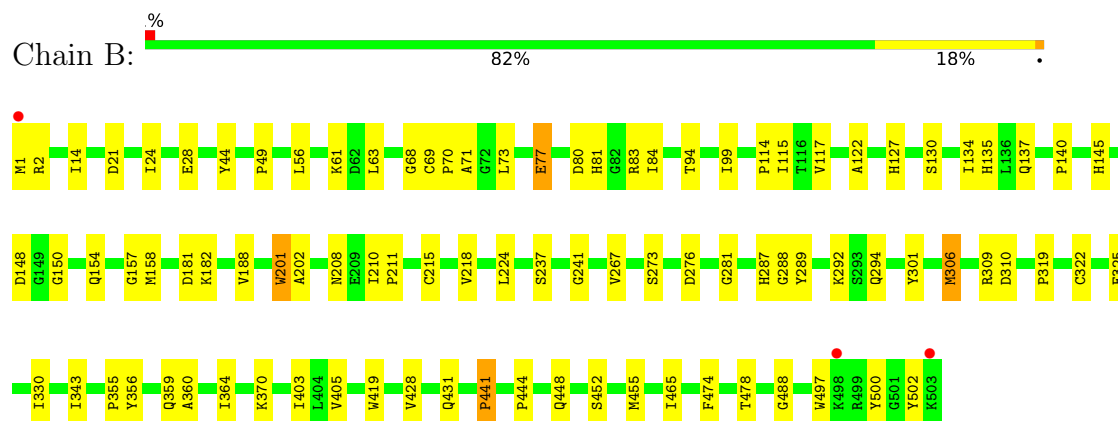
3 Residue-property plots

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.

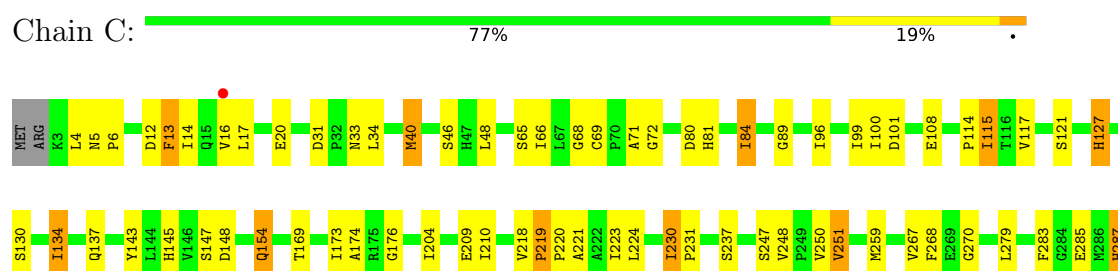
• Molecule 1: Ferulic acid decarboxylase 1

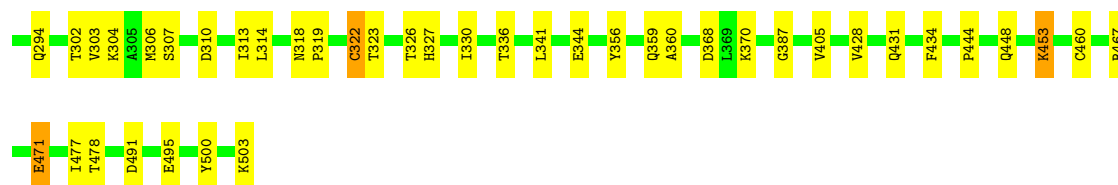


• Molecule 1: Ferulic acid decarboxylase 1

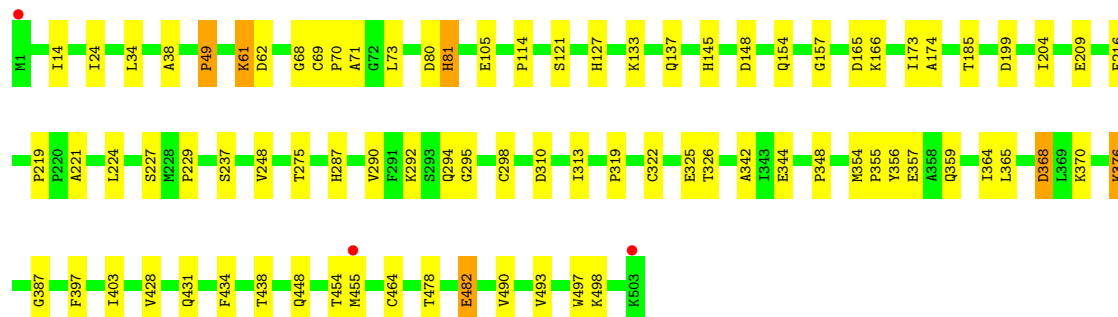
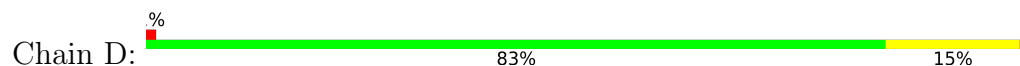


• Molecule 1: Ferulic acid decarboxylase 1





• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.163 , 0.192 (Not available) , 0.193	Depositor DCC
R_{free} test set	15010 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: 4LU, K, MN, NA

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	1.73	25/4152 (0.6%)	1.44	5/5637 (0.1%)
1	B	1.74	39/4133 (0.9%)	1.42	13/5612 (0.2%)
1	C	1.80	53/4078 (1.3%)	1.48	17/5542 (0.3%)
1	D	1.71	37/4132 (0.9%)	1.42	6/5611 (0.1%)
All	All	1.74	154/16495 (0.9%)	1.44	41/22402 (0.2%)

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	81	HIS	N-CA	9.43	1.56	1.46
1	B	343	ILE	CA-CB	-8.65	1.43	1.54
1	C	360	ALA	CA-CB	8.51	1.67	1.53
1	D	157	GLY	N-CA	8.43	1.52	1.44
1	B	478	THR	CA-CB	7.98	1.64	1.53
1	D	370	LYS	N-CA	7.63	1.55	1.46
1	B	360	ALA	CA-CB	7.55	1.65	1.53
1	D	133	LYS	CA-C	7.42	1.63	1.52
1	C	405	VAL	N-CA	7.40	1.54	1.46
1	A	66	ILE	N-CA	7.38	1.54	1.46
1	D	204	ILE	CA-CB	7.24	1.64	1.54
1	A	477	ILE	CA-CB	7.21	1.62	1.54
1	A	270	GLY	N-CA	7.20	1.53	1.45
1	D	478	THR	N-CA	7.20	1.55	1.46
1	D	73	LEU	N-CA	7.17	1.54	1.45
1	A	168	TRP	N-CA	7.10	1.54	1.46
1	A	344	GLU	CA-C	-7.10	1.43	1.52
1	C	84	ILE	CA-CB	7.05	1.62	1.54
1	B	474	PHE	CA-C	-6.96	1.46	1.53
1	D	493	VAL	CA-CB	6.89	1.63	1.54
1	C	72	GLY	N-CA	6.86	1.53	1.45
1	A	292	LYS	N-CA	6.84	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	229	PRO	CA-C	6.82	1.58	1.53
1	A	288	GLY	N-CA	6.80	1.54	1.45
1	C	503	LYS	CA-CB	6.79	1.67	1.53
1	C	66	ILE	C-O	6.45	1.31	1.24
1	D	326	THR	C-O	6.42	1.32	1.24
1	D	34	LEU	N-CA	6.30	1.54	1.46
1	B	241	GLY	N-CA	6.22	1.53	1.45
1	D	216	PHE	CA-C	-6.19	1.45	1.52
1	D	313	ILE	CA-CB	-6.18	1.46	1.54
1	D	490	VAL	CA-CB	-6.17	1.47	1.54
1	B	288	GLY	N-CA	6.13	1.54	1.45
1	C	368	ASP	N-CA	6.13	1.53	1.46
1	C	101	ASP	N-CA	-6.11	1.38	1.46
1	D	298	CYS	N-CA	-6.10	1.41	1.46
1	C	169	THR	N-CA	-6.10	1.39	1.46
1	B	157	GLY	N-CA	6.08	1.50	1.44
1	B	68	GLY	N-CA	6.07	1.53	1.44
1	D	185	THR	C-O	-6.05	1.16	1.23
1	A	157	GLY	N-CA	6.04	1.50	1.44
1	C	174	ALA	CA-C	-6.02	1.45	1.52
1	B	215	CYS	N-CA	6.02	1.53	1.46
1	D	365	LEU	N-CA	6.01	1.53	1.46
1	C	304	LYS	N-CA	6.00	1.53	1.45
1	B	301	TYR	N-CA	-5.97	1.38	1.46
1	D	354	MET	N-CA	5.96	1.52	1.46
1	C	230	ILE	CA-CB	5.95	1.61	1.54
1	C	33	ASN	CA-C	5.94	1.60	1.52
1	C	121	SER	CA-C	5.94	1.61	1.52
1	C	478	THR	CA-CB	5.94	1.61	1.53
1	C	322	CYS	CA-C	5.91	1.60	1.52
1	C	69	CYS	CA-CB	5.91	1.62	1.53
1	D	199	ASP	CA-C	5.88	1.60	1.52
1	A	202	ALA	CA-CB	5.87	1.62	1.53
1	B	292	LYS	CA-C	-5.86	1.45	1.52
1	C	327	HIS	N-CA	5.86	1.53	1.46
1	C	13	PHE	CA-CB	5.83	1.62	1.53
1	A	430	ASP	CG-OD1	5.82	1.36	1.25
1	C	313	ILE	C-O	-5.81	1.17	1.24
1	B	117	VAL	N-CA	5.81	1.51	1.46
1	B	355	PRO	CA-CB	5.81	1.61	1.53
1	C	318	ASN	CA-C	5.81	1.58	1.52
1	A	197	ILE	CA-C	5.79	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	TYR	CA-C	5.75	1.59	1.52
1	B	14	ILE	CA-C	5.72	1.59	1.52
1	C	6	PRO	C-O	-5.71	1.16	1.24
1	A	294	GLN	CD-OE1	5.71	1.34	1.23
1	B	309	ARG	N-CA	5.67	1.53	1.45
1	C	31	ASP	CA-C	5.65	1.58	1.52
1	A	292	LYS	CA-C	-5.64	1.45	1.52
1	D	68	GLY	N-CA	5.64	1.51	1.45
1	D	221	ALA	CA-CB	5.64	1.62	1.53
1	C	230	ILE	N-CA	-5.63	1.39	1.46
1	B	140	PRO	N-CA	5.61	1.51	1.47
1	B	465	ILE	CA-CB	-5.59	1.47	1.54
1	D	165	ASP	N-CA	5.58	1.53	1.46
1	A	44	TYR	N-CA	5.57	1.53	1.46
1	C	250	VAL	N-CA	-5.56	1.40	1.46
1	C	267	VAL	N-CA	5.56	1.52	1.46
1	D	403	ILE	CA-C	5.54	1.59	1.52
1	B	405	VAL	N-CA	5.53	1.52	1.46
1	A	248	VAL	CA-CB	5.53	1.63	1.54
1	C	34	LEU	N-CA	5.52	1.53	1.46
1	C	341	LEU	C-O	-5.52	1.17	1.24
1	C	259	MET	N-CA	5.52	1.52	1.46
1	C	176	GLY	N-CA	5.51	1.53	1.45
1	A	503	LYS	CA-CB	5.50	1.64	1.53
1	A	15	GLN	N-CA	5.50	1.53	1.46
1	D	295	GLY	C-O	5.50	1.31	1.23
1	C	89	GLY	N-CA	5.49	1.53	1.45
1	B	267	VAL	N-CA	5.47	1.52	1.46
1	D	482	GLU	CG-CD	5.47	1.65	1.52
1	B	63	LEU	N-CA	5.45	1.53	1.46
1	C	99	ILE	CA-CB	-5.45	1.48	1.54
1	A	161	LEU	N-CA	5.45	1.52	1.45
1	C	318	ASN	N-CA	-5.45	1.40	1.46
1	B	452	SER	CA-C	5.43	1.60	1.52
1	B	150	GLY	N-CA	5.39	1.51	1.45
1	A	140	PRO	CA-CB	5.38	1.59	1.53
1	C	100	ILE	CA-CB	5.37	1.61	1.54
1	D	357	GLU	N-CA	5.35	1.53	1.46
1	D	397	PHE	N-CA	5.33	1.52	1.46
1	C	219	PRO	CA-CB	-5.31	1.46	1.54
1	C	247	SER	N-CA	5.31	1.52	1.46
1	C	127	HIS	N-CA	-5.30	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	ILE	CA-CB	-5.29	1.48	1.54
1	C	500	TYR	N-CA	5.29	1.52	1.46
1	A	285	GLU	CA-C	5.28	1.60	1.53
1	D	121	SER	CA-C	5.28	1.59	1.52
1	B	309	ARG	CD-NE	5.28	1.53	1.46
1	B	154	GLN	CA-CB	5.27	1.60	1.52
1	C	115	ILE	CA-CB	5.26	1.60	1.54
1	B	94	THR	CA-CB	5.26	1.61	1.53
1	B	488	GLY	N-CA	5.26	1.52	1.45
1	C	143	TYR	CA-C	5.26	1.59	1.53
1	D	348	PRO	CA-C	5.26	1.57	1.53
1	C	71	ALA	CA-CB	5.25	1.60	1.53
1	D	438	THR	CA-C	5.25	1.59	1.52
1	C	65	SER	N-CA	5.24	1.52	1.45
1	C	221	ALA	CA-C	5.23	1.59	1.52
1	A	338	ALA	N-CA	5.22	1.52	1.46
1	B	218	VAL	CA-CB	5.22	1.60	1.54
1	D	464	CYS	C-O	-5.22	1.16	1.23
1	B	281	GLY	N-CA	5.20	1.51	1.44
1	B	99	ILE	N-CA	5.20	1.52	1.46
1	A	344	GLU	C-O	5.19	1.30	1.24
1	C	5	ASN	CA-C	5.18	1.58	1.52
1	C	40	MET	CA-C	5.18	1.59	1.52
1	C	287	HIS	N-CA	5.17	1.52	1.46
1	D	292	LYS	N-CA	5.16	1.52	1.46
1	D	497	TRP	N-CA	5.15	1.52	1.46
1	C	267	VAL	CA-CB	-5.14	1.48	1.54
1	C	477	ILE	CA-CB	5.13	1.60	1.54
1	C	370	LYS	C-O	-5.13	1.18	1.24
1	B	73	LEU	N-CA	5.13	1.52	1.45
1	D	342	ALA	CA-CB	5.11	1.61	1.53
1	A	188	VAL	CA-C	5.11	1.59	1.52
1	B	135	HIS	C-O	-5.10	1.16	1.23
1	A	186	GLY	N-CA	5.09	1.50	1.45
1	C	66	ILE	N-CA	5.08	1.52	1.46
1	B	292	LYS	N-CA	5.08	1.52	1.46
1	C	154	GLN	CA-C	5.05	1.59	1.53
1	A	81	HIS	N-CA	5.05	1.52	1.46
1	B	364	ILE	CA-CB	5.04	1.60	1.54
1	B	419	TRP	N-CA	5.04	1.52	1.46
1	C	204	ILE	CA-CB	5.04	1.60	1.54
1	D	295	GLY	N-CA	5.03	1.51	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	VAL	C-O	5.03	1.30	1.24
1	D	292	LYS	CA-C	-5.03	1.46	1.52
1	B	182	LYS	CD-CE	5.02	1.67	1.52
1	B	56	LEU	CA-C	-5.02	1.46	1.52
1	B	465	ILE	N-CA	5.01	1.52	1.46
1	C	134	ILE	N-CA	5.01	1.52	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ILE	N-CA-C	-8.31	102.44	110.42
1	B	122	ALA	CA-C-O	6.85	125.90	119.59
1	B	330	ILE	N-CA-C	-6.75	104.18	110.53
1	C	14	ILE	N-CA-C	-6.39	104.26	110.72
1	C	117	VAL	CA-C-N	-6.36	113.43	119.85
1	C	117	VAL	C-N-CA	-6.36	113.43	119.85
1	D	248	VAL	CB-CA-C	-6.32	104.07	110.89
1	C	314	LEU	CA-C-N	-6.19	113.58	120.14
1	C	314	LEU	C-N-CA	-6.19	113.58	120.14
1	C	336	THR	N-CA-C	6.19	118.54	111.11
1	C	223	ILE	N-CA-C	-6.09	103.47	111.09
1	C	248	VAL	N-CA-C	-6.00	103.07	108.95
1	C	143	TYR	N-CA-C	-5.71	97.12	107.75
1	B	201	TRP	N-CA-C	-5.63	105.39	111.53
1	D	174	ALA	N-CA-C	-5.59	99.19	108.75
1	A	41	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	B	403	ILE	N-CA-CB	-5.56	103.69	111.25
1	B	83	ARG	NE-CZ-NH2	-5.54	114.22	119.20
1	A	117	VAL	CA-C-N	-5.53	114.26	119.85
1	A	117	VAL	C-N-CA	-5.53	114.26	119.85
1	A	293	SER	N-CA-C	-5.53	105.17	112.24
1	C	210	ILE	O-C-N	5.48	126.33	121.57
1	C	147	SER	N-CA-C	5.46	119.76	113.38
1	C	20	GLU	N-CA-C	-5.45	105.85	112.88
1	C	100	ILE	CA-C-O	5.38	126.55	120.95
1	D	368	ASP	CA-C-O	5.36	126.66	120.60
1	B	115	ILE	CA-C-O	5.35	126.15	120.48
1	C	303	VAL	O-C-N	5.32	129.43	122.94
1	B	202	ALA	N-CA-C	-5.28	105.53	111.28
1	D	38	ALA	N-CA-C	5.21	117.04	111.36
1	C	210	ILE	CA-C-N	-5.21	114.59	119.85
1	C	210	ILE	C-N-CA	-5.21	114.59	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	PRO	CB-CA-C	-5.13	104.38	111.21
1	B	441	PRO	CB-CA-C	-5.08	104.26	111.68
1	B	44	TYR	CB-CA-C	-5.07	102.37	110.79
1	A	38	ALA	N-CA-C	5.06	116.80	111.28
1	B	158	MET	N-CA-CB	-5.05	102.62	110.55
1	B	276	ASP	N-CA-C	-5.03	99.08	108.02
1	D	209	GLU	CA-C-N	-5.01	117.81	123.02
1	D	209	GLU	C-N-CA	-5.01	117.81	123.02
1	C	130	SER	N-CA-C	-5.00	102.62	110.17

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	46	0
1	B	4032	0	4021	39	0
1	C	3975	0	3963	46	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	5	0
5	B	36	0	28	6	0
5	C	36	0	27	6	0
5	D	36	0	28	4	0
6	A	437	0	0	23	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	358	0	0	12	1
6	C	275	0	0	6	0
6	D	377	0	0	14	0
All	All	17693	0	16169	188	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 6.

All (188) 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	1.35
1:D:368:ASP:CG	6:D:701:HOH:O	1.77	1.26
1:B:28[B]:GLU:OE2	6:B:701:HOH:O	1.56	1.22
5:A:604:4LU:H14	5:A:604:4LU:H5	1.46	0.97
1:A:483:LYS:HE3	6:A:957:HOH:O	1.65	0.97
5:C:603:4LU:H5	5:C:603:4LU:H14	1.48	0.93
5:D:603:4LU:H14	5:D:603:4LU:H5	1.52	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
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
1:A:344:GLU:HG3	6:A:1057:HOH:O	1.86	0.76
5:B:604:4LU:H5	5:B:604:4LU:H14	1.68	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:B:455:MET:HE1	6:B:765:HOH:O	1.88	0.73
1:C:428:VAL:H	1:C:431:GLN:HE21	1.35	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:C:603:4LU:H14	5:C:603:4LU:C13	2.22	0.70
1:A:5:ASN:OD1	6:A:702:HOH:O	2.09	0.69
5:D:603:4LU:H14	5:D:603:4LU:C13	2.21	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
5:A:604:4LU:H14	5:A:604:4LU:C13	2.21	0.68
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: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:C:145:HIS:HD2	1:C:148:ASP:OD2	1.83	0.62
5:A:604:4LU:C13	5:A:604:4LU:C7M	2.78	0.61
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
5:A:604:4LU:H5	5:A:604:4LU:C7M	2.26	0.60
1:C:224:LEU:C	1:C:224:LEU:HD23	2.27	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:O4	5:B:604:4LU:H6	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
5:C:603:4LU:H5	5:C:603:4LU:C7M	2.28	0.58

Continued on next page...

Continued from previous page...

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
5:C:603:4LU:C13	5:C:603:4LU:C7M	2.81	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
5:D:603:4LU:C13	5:D:603:4LU:C7M	2.83	0.56
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:A:430:ASP:CB	6:A:701:HOH:O	2.32	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:84:ILE:HD12	1:C:84:ILE:H	1.73	0.53
1:C:283:PHE:O	1:C:285[B]:GLU:HG3	2.07	0.53
1:D:105:GLU:CD	6:D:707:HOH:O	2.52	0.53
1:C:467:ARG:NH2	1:C:471:GLU:OE2	2.41	0.53
1:B:441:PRO:HB3	1:B:455:MET:HE3	1.91	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:268:PHE:CZ	1:C:306[A]:MET:HE3	2.46	0.51
1:C:4:LEU:CD1	1:C:16[B]:VAL:HG12	2.41	0.50
5:B:604:4LU:H14	5:B:604:4LU:C13	2.37	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ARG:HG3	1:C:467:ARG:NH2	2.29	0.48
5:C:603:4LU:O4	5:C:603:4LU:H6	2.14	0.47
5:B:604:4LU:H22	5:B:604:4LU:H7	1.78	0.47
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:173:ILE:HD12	5:C:603:4LU:H18	1.96	0.47
1:B:28[B]:GLU:H	1:B:28[B]:GLU:CD	2.22	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:D:224:LEU:C	1:D:224:LEU:HD23	2.41	0.46
5:B:604:4LU:H17	5:B:604:4LU:H16	1.72	0.46
1:C:40:MET:HE3	1:C:68:GLY:CA	2.45	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:D:455[C]:MET:HE3	1:D:455[C]:MET:HA	2.00	0.44
5:B:604:4LU:C13	5:B:604:4LU:C7M	2.96	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:A:134:ILE:CD1	1:A:306[B]:MET:HE3	2.48	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:251:VAL:CG2	6:C:944:HOH:O	2.67	0.42
1:C:431:GLN:HB3	1:C:460[B]:CYS:SG	2.59	0.42
1:D:62:ASP:CG	6:D:706:HOH:O	2.61	0.42
1:B:201:TRP:CB	1:B:210:ILE:HG12	2.50	0.42
1:B:224:LEU:C	1:B:224:LEU:HD23	2.44	0.42
1:D:275:THR:HG21	6:D:887:HOH:O	2.19	0.42
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:B:455:MET:HG3	6:B:919:HOH:O	2.19	0.41
1:C:306[B]:MET:HB2	1:C:306[B]:MET:HE2	1.62	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:69:CYS:N	1:B:70:PRO:HD2	2.36	0.41
1:B:114:PRO:HG3	1:B:237:SER:HB2	2.01	0.41
1:C:46:SER:HB2	1:C:48:LEU:HG	2.02	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: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:134:ILE:HD13	1:C:306[B]:MET:HE3	2.03	0.40
1:C:209:GLU:HG3	1:C:209:GLU:O	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:24:ILE:HG12	1:D:49:PRO:HB2	2.02	0.40
1:D:322:CYS:N	1:D:359:GLN:HE22	2.15	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 ⓘ

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	515/503 (102%)	506 (98%)	9 (2%)	0	100	100
1	B	512/503 (102%)	497 (97%)	14 (3%)	1 (0%)	43	27
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%)	445 (99%)	6 (1%)	61	42
1	B	447/438 (102%)	441 (99%)	6 (1%)	61	42
1	C	441/438 (101%)	431 (98%)	10 (2%)	44	21
1	D	449/438 (102%)	442 (98%)	7 (2%)	55	34
All	All	1788/1752 (102%)	1759 (98%)	29 (2%)	55	34

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

Mol	Chain	Res	Type
1	A	61	LYS
1	A	78	LYS
1	A	132	GLU
1	A	137	GLN
1	A	181	ASP
1	A	220	PRO
1	B	61	LYS
1	B	77	GLU
1	B	181	ASP
1	B	306[A]	MET
1	B	306[B]	MET
1	B	370	LYS
1	C	96	ILE
1	C	108	GLU
1	C	115	ILE
1	C	137	GLN
1	C	154	GLN
1	C	220	PRO
1	C	251	VAL
1	C	279	LEU
1	C	453	LYS
1	C	471	GLU
1	D	49	PRO
1	D	61	LYS
1	D	137	GLN
1	D	154	GLN
1	D	219	PRO
1	D	376	LYS
1	D	498	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	81	HIS
1	A	127	HIS
1	A	145	HIS
1	A	162	GLN
1	A	287	HIS
1	A	294	GLN
1	A	296	HIS
1	A	359	GLN
1	A	431	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	33	ASN
1	B	81	HIS
1	B	127	HIS
1	B	145	HIS
1	B	162	GLN
1	B	287	HIS
1	B	296	HIS
1	B	359	GLN
1	B	431	GLN
1	B	448	GLN
1	C	33	ASN
1	C	81	HIS
1	C	127	HIS
1	C	137	GLN
1	C	145	HIS
1	C	162	GLN
1	C	287	HIS
1	C	311	ASN
1	C	359	GLN
1	C	431	GLN
1	C	448	GLN
1	D	33	ASN
1	D	81	HIS
1	D	127	HIS
1	D	145	HIS
1	D	162	GLN
1	D	287	HIS
1	D	296	HIS
1	D	311	ASN
1	D	359	GLN
1	D	431	GLN
1	D	448	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	604	3,4	35,39,39	1.70	9 (25%)	44,62,62	2.32	17 (38%)
5	4LU	D	603	3,4	35,39,39	1.57	7 (20%)	44,62,62	1.97	9 (20%)
5	4LU	C	603	3,4	35,39,39	2.68	11 (31%)	44,62,62	2.37	17 (38%)
5	4LU	B	604	3,4	35,39,39	1.92	11 (31%)	44,62,62	2.62	16 (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	A	604	3,4	-	2/18/30/30	0/4/4/4
5	4LU	D	603	3,4	-	1/18/30/30	0/4/4/4
5	4LU	C	603	3,4	-	5/18/30/30	0/4/4/4
5	4LU	B	604	3,4	-	3/18/30/30	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	603	4LU	C2'-C3'	-7.25	1.40	1.53
5	C	603	4LU	C5'-C4'	6.69	1.60	1.51
5	C	603	4LU	C4'-C3'	-5.70	1.43	1.53
5	C	603	4LU	C4-N3	5.10	1.48	1.38
5	B	604	4LU	C5A-C6	4.51	1.44	1.39
5	A	604	4LU	C2'-C3'	-4.28	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	603	4LU	C2'-C3'	-4.14	1.46	1.53
5	B	604	4LU	C3-C5	-4.04	1.48	1.54
5	B	604	4LU	C4-N3	3.99	1.46	1.38
5	C	603	4LU	C10-N1	3.61	1.43	1.37
5	C	603	4LU	C5A-C6	3.53	1.43	1.39
5	D	603	4LU	C3-C5	-3.49	1.49	1.54
5	A	604	4LU	C2-N3	-3.46	1.31	1.37
5	C	603	4LU	C2-N3	-3.28	1.32	1.37
5	A	604	4LU	C7M-C7	3.26	1.58	1.51
5	C	603	4LU	O3'-C3'	3.24	1.51	1.43
5	A	604	4LU	C5A-C6	3.06	1.42	1.39
5	C	603	4LU	C3-C5	-2.87	1.50	1.54
5	B	604	4LU	C5-C6	-2.87	1.42	1.54
5	B	604	4LU	C5'-C4'	2.87	1.55	1.51
5	D	603	4LU	C9-C8	2.73	1.43	1.39
5	D	603	4LU	C5A-C6	2.67	1.42	1.39
5	A	604	4LU	C10-N10	-2.66	1.33	1.38
5	A	604	4LU	C5'-C4'	2.64	1.55	1.51
5	A	604	4LU	C3-C5	-2.54	1.50	1.54
5	B	604	4LU	C2-N3	-2.52	1.33	1.37
5	B	604	4LU	C4A-C4	-2.46	1.36	1.43
5	D	603	4LU	C8M-C8	-2.46	1.46	1.51
5	B	604	4LU	C9-C9A	2.46	1.43	1.39
5	C	603	4LU	C9-C8	2.45	1.42	1.39
5	B	604	4LU	C9-C8	2.44	1.42	1.39
5	C	603	4LU	C5-C6	-2.41	1.44	1.54
5	D	603	4LU	C4-N3	2.37	1.43	1.38
5	A	604	4LU	C5-C6	-2.34	1.44	1.54
5	A	604	4LU	C13-C5	2.20	1.59	1.53
5	D	603	4LU	C5'-C4'	2.15	1.54	1.51
5	B	604	4LU	C4'-C3'	-2.13	1.49	1.53
5	B	604	4LU	C8M-C8	-2.09	1.47	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	4LU	C9-C8-C7	6.63	125.79	119.10
5	C	603	4LU	O4-C4-N3	-5.80	109.21	120.11
5	B	604	4LU	C4A-C10-N10	5.50	124.02	119.02
5	B	604	4LU	O4-C4-N3	-5.45	109.86	120.11
5	B	604	4LU	C5-C6-C5A	-5.27	115.72	121.48
5	D	603	4LU	C4-N3-C2	-5.25	119.13	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604	4LU	C12-C5-C13	-5.19	97.14	108.63
5	A	604	4LU	C5'-C4'-C3'	-5.19	102.42	112.22
5	D	603	4LU	C4A-C4-N3	5.09	122.37	111.84
5	B	604	4LU	C4-N3-C2	-5.05	119.41	126.37
5	B	604	4LU	C7M-C7-C8	-5.03	110.98	119.67
5	B	604	4LU	C4A-C4-N3	4.84	121.84	111.84
5	C	603	4LU	C4-N3-C2	-4.80	119.75	126.37
5	D	603	4LU	C5-C6-C5A	-4.69	116.36	121.48
5	C	603	4LU	C4A-C4-N3	4.57	121.28	111.84
5	C	603	4LU	C4'-C3'-C2'	4.37	120.84	113.57
5	A	604	4LU	C4A-C4-N3	4.32	120.78	111.84
5	C	603	4LU	C5'-C4'-C3'	-4.29	104.12	112.22
5	A	604	4LU	O4-C4-N3	-4.27	112.08	120.11
5	B	604	4LU	C8-C7-C6	4.17	123.22	119.50
5	A	604	4LU	O2'-C2'-C3'	4.00	118.61	109.25
5	D	603	4LU	O4-C4-N3	-3.89	112.80	120.11
5	A	604	4LU	C8M-C8-C9	-3.69	113.07	119.57
5	C	603	4LU	O4'-C4'-C3'	3.66	117.82	109.25
5	C	603	4LU	C9-C8-C7	3.58	122.72	119.10
5	C	603	4LU	O3'-C3'-C2'	3.57	117.03	108.93
5	A	604	4LU	C12-C5-C3	3.43	114.80	109.50
5	A	604	4LU	C4-N3-C2	-3.36	121.74	126.37
5	B	604	4LU	C13-C5-C3	-3.35	104.33	109.50
5	B	604	4LU	C8M-C8-C7	3.14	125.62	121.18
5	D	603	4LU	O4'-C4'-C5'	-3.12	103.10	109.99
5	C	603	4LU	C4A-C10-N10	3.06	121.80	119.02
5	D	603	4LU	C5'-C4'-C3'	-2.99	106.57	112.22
5	C	603	4LU	N1-C2-N3	2.97	120.41	115.74
5	B	604	4LU	C8M-C8-C9	-2.97	114.34	119.57
5	A	604	4LU	O2-C2-N3	-2.95	116.62	121.86
5	A	604	4LU	O3'-C3'-C4'	2.84	115.39	108.93
5	A	604	4LU	C12-C5-C13	-2.84	102.36	108.63
5	B	604	4LU	C3-C5-C6	2.78	113.74	107.38
5	D	603	4LU	C13-C5-C6	2.73	120.14	112.06
5	C	603	4LU	C2'-C1'-N10	2.68	122.86	110.20
5	D	603	4LU	C12-C5-C13	-2.67	102.72	108.63
5	C	603	4LU	O2'-C2'-C3'	2.67	115.49	109.25
5	C	603	4LU	C5-C6-C5A	-2.64	118.59	121.48
5	A	604	4LU	C5-C6-C5A	-2.63	118.61	121.48
5	B	604	4LU	C13-C5-C6	2.54	119.60	112.06
5	D	603	4LU	C9-C8-C7	2.52	121.64	119.10
5	B	604	4LU	O2'-C2'-C3'	-2.51	103.38	109.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604	4LU	O3'-C3'-C2'	-2.48	103.30	108.93
5	B	604	4LU	C5'-C4'-C3'	-2.44	107.61	112.22
5	C	603	4LU	O1P-P-O3P	2.32	116.50	107.80
5	A	604	4LU	C2'-C1'-N10	2.30	121.09	110.20
5	A	604	4LU	O3'-C3'-C2'	2.25	114.04	108.93
5	A	604	4LU	O5'-C5'-C4'	-2.18	103.53	109.36
5	A	604	4LU	N1-C2-N3	2.18	119.16	115.74
5	C	603	4LU	C13-C5-C3	-2.18	106.15	109.50
5	C	603	4LU	C8M-C8-C9	-2.13	115.82	119.57
5	A	604	4LU	C5A-C6-C7	-2.10	114.58	118.00
5	C	603	4LU	C5A-C6-C7	-2.03	114.69	118.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	4LU	C2'-C1'-N10-C10
5	B	604	4LU	C2'-C1'-N10-C10
5	D	603	4LU	C2'-C1'-N10-C10
5	C	603	4LU	O3'-C3'-C4'-C5'
5	C	603	4LU	O3'-C3'-C4'-O4'
5	B	604	4LU	C2'-C3'-C4'-C5'
5	C	603	4LU	C2'-C1'-N10-C10
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

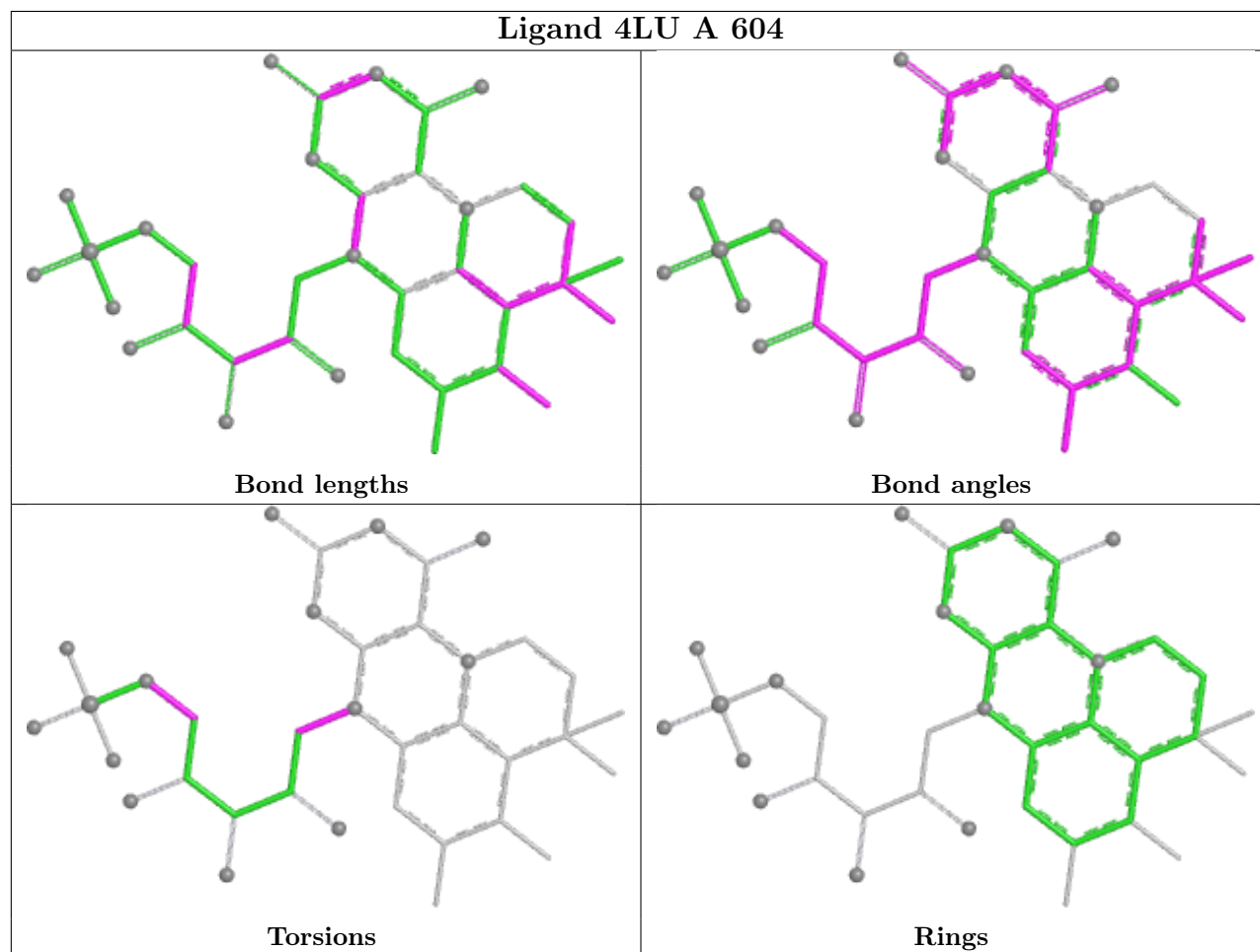
There are no ring outliers.

4 monomers are involved in 21 short contacts:

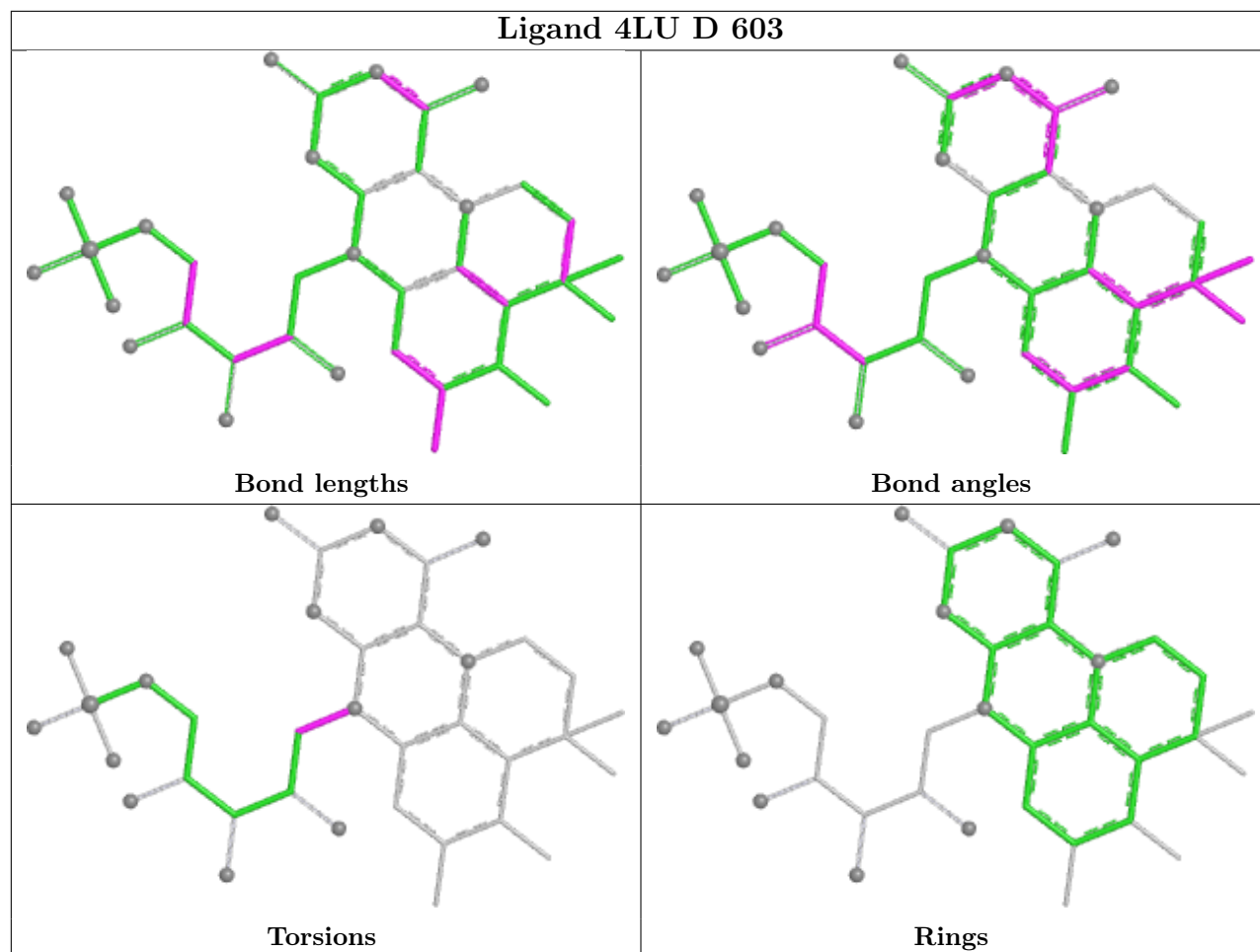
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	4LU	5	0
5	D	603	4LU	4	0
5	C	603	4LU	6	0
5	B	604	4LU	6	0

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.

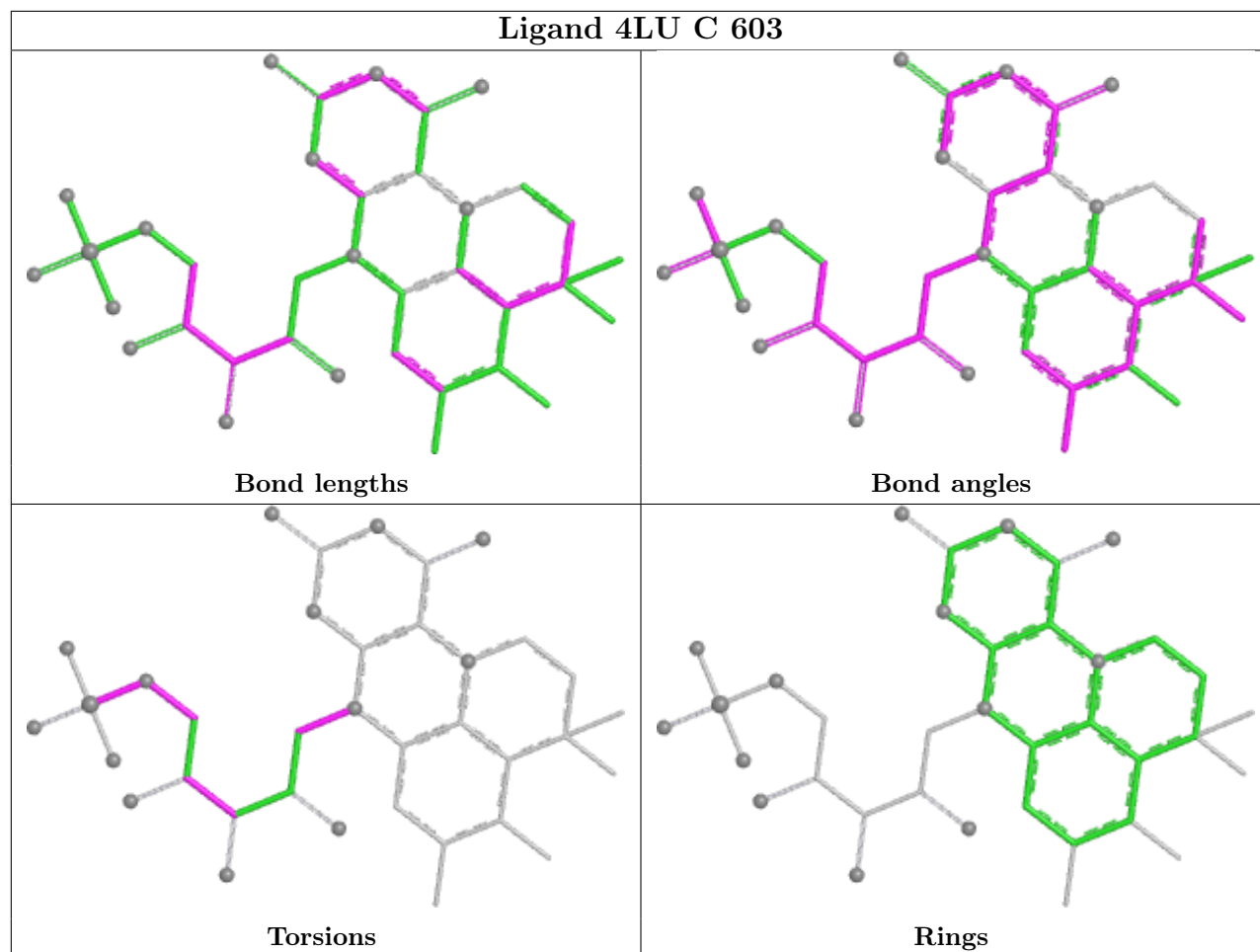
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

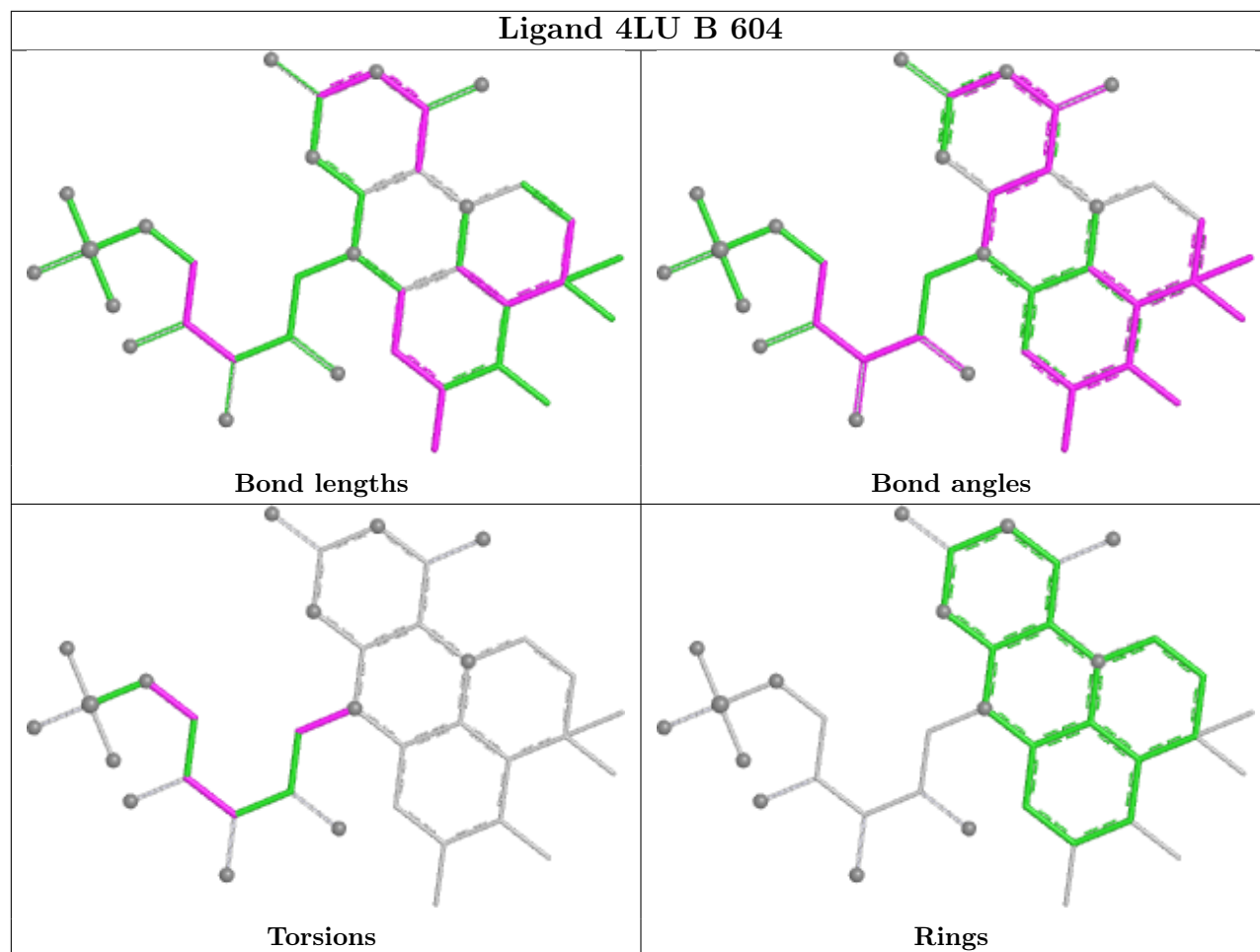


Ligand 4LU D 603



Ligand 4LU C 603





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	503/503 (100%)	-0.50	2 (0%) 88 92	7, 20, 33, 46	14 (2%)
1	B	503/503 (100%)	-0.38	3 (0%) 85 90	8, 21, 38, 62	11 (2%)
1	C	501/503 (99%)	-0.02	1 (0%) 91 93	9, 26, 40, 57	9 (1%)
1	D	503/503 (100%)	-0.39	3 (0%) 85 90	8, 22, 36, 66	12 (2%)
All	All	2010/2012 (99%)	-0.32	9 (0%) 88 92	7, 22, 38, 66	46 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	GLY	3.0
1	D	503	LYS	3.0
1	B	503	LYS	2.6
1	D	1	MET	2.5
1	C	16[A]	VAL	2.3
1	A	293	SER	2.3
1	B	1	MET	2.2
1	D	455[A]	MET	2.2
1	B	498	LYS	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 oligosaccharides in this entry.

6.4 Ligands

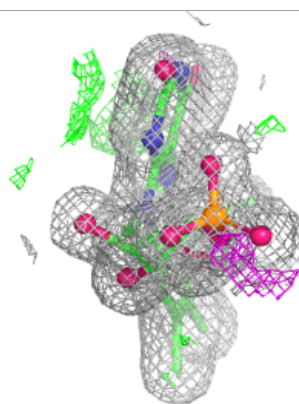
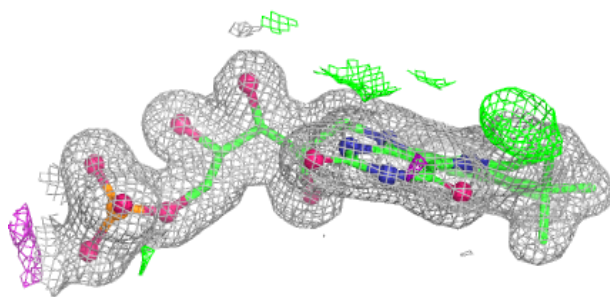
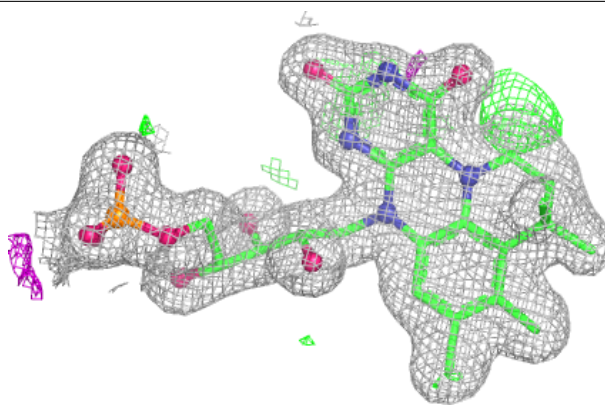
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NA	C	604	1/1	0.88	0.09	38,38,38,38	0
2	NA	B	601	1/1	0.97	0.05	22,22,22,22	0
2	NA	A	601	1/1	0.97	0.05	27,27,27,27	0
5	4LU	C	603	36/36	0.97	0.06	17,21,28,30	0
5	4LU	A	604	36/36	0.98	0.05	13,15,24,28	0
5	4LU	B	604	36/36	0.98	0.05	13,17,24,26	0
3	K	C	602	1/1	0.98	0.04	21,21,21,21	0
5	4LU	D	603	36/36	0.98	0.04	15,18,24,27	0
4	MN	C	601	1/1	0.99	0.04	21,21,21,21	1
3	K	B	602	1/1	1.00	0.03	16,16,16,16	0
4	MN	D	601	1/1	1.00	0.03	20,20,20,20	1
3	K	A	602	1/1	1.00	0.02	15,15,15,15	0
3	K	D	602	1/1	1.00	0.02	18,18,18,18	0
4	MN	A	603	1/1	1.00	0.02	16,16,16,16	1
4	MN	B	603	1/1	1.00	0.03	17,17,17,17	1

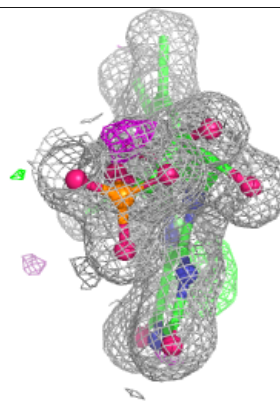
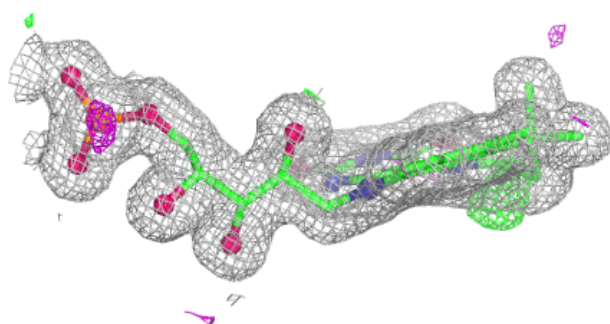
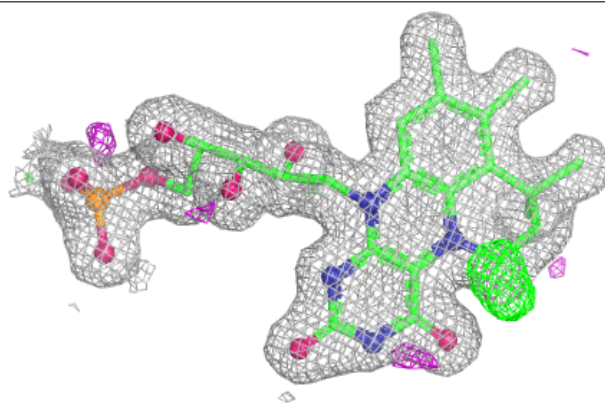
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4LU 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)

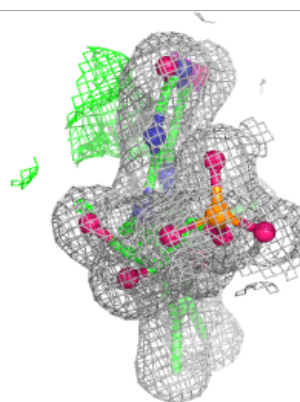
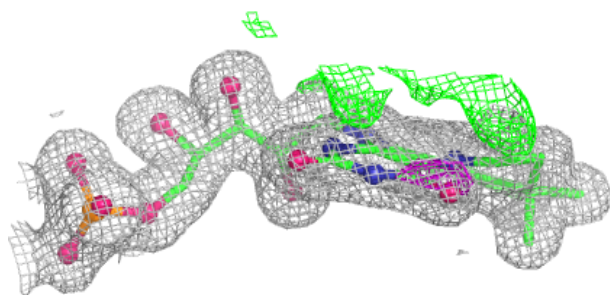
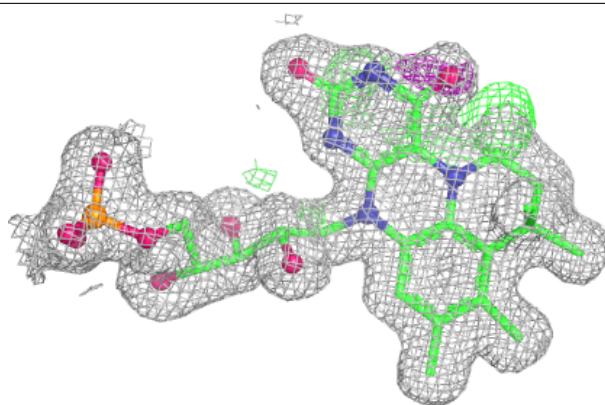
**Electron density around 4LU A 604:**

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

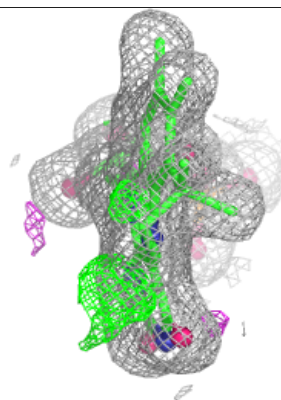
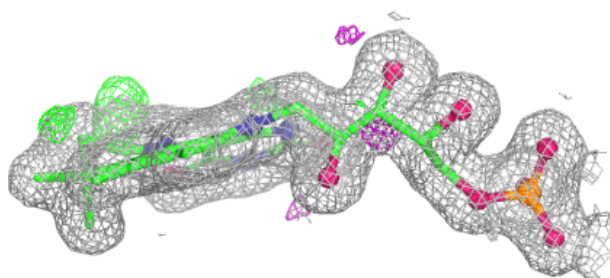
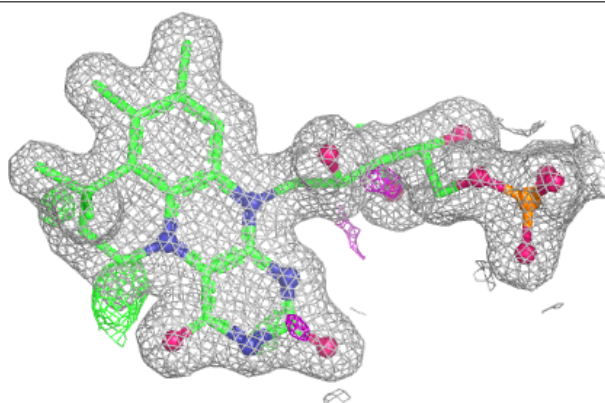


Electron density around 4LU B 604:

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

**Electron density around 4LU 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.