Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 03:29 PM JST

PDB ID	:	5JJQ
Title	:	Crystal structure of IdnL1
Authors	:	Cieslak, J.; Miyanaga, A.; Kudo, F.; Eguchi, T.
Deposited on	:	2016-04-25
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

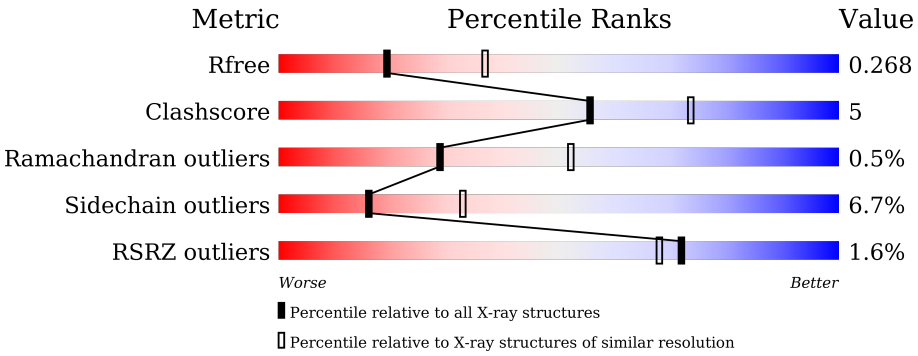
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	552	2% 75% 12% • 12%
1	B	552	% 73% 13% • 12%
1	C	552	% 74% 13% • 11%
1	D	552	2% 71% 15% • 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15125 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 AMP-dependent synthetase and ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	1	0
			3685	2335	655	684	11			
1	B	487	Total	C	N	O	S	0	1	0
			3685	2339	654	681	11			
1	C	489	Total	C	N	O	S	0	1	0
			3697	2341	659	686	11			
1	D	487	Total	C	N	O	S	0	1	0
			3691	2340	657	683	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A077KT11
A	-18	GLY	-	expression tag	UNP A0A077KT11
A	-17	SER	-	expression tag	UNP A0A077KT11
A	-16	SER	-	expression tag	UNP A0A077KT11
A	-15	HIS	-	expression tag	UNP A0A077KT11
A	-14	HIS	-	expression tag	UNP A0A077KT11
A	-13	HIS	-	expression tag	UNP A0A077KT11
A	-12	HIS	-	expression tag	UNP A0A077KT11
A	-11	HIS	-	expression tag	UNP A0A077KT11
A	-10	HIS	-	expression tag	UNP A0A077KT11
A	-9	SER	-	expression tag	UNP A0A077KT11
A	-8	SER	-	expression tag	UNP A0A077KT11
A	-7	GLY	-	expression tag	UNP A0A077KT11
A	-6	LEU	-	expression tag	UNP A0A077KT11
A	-5	VAL	-	expression tag	UNP A0A077KT11
A	-4	PRO	-	expression tag	UNP A0A077KT11
A	-3	ARG	-	expression tag	UNP A0A077KT11
A	-2	GLY	-	expression tag	UNP A0A077KT11
A	-1	SER	-	expression tag	UNP A0A077KT11
A	0	HIS	-	expression tag	UNP A0A077KT11
B	-19	MET	-	initiating methionine	UNP A0A077KT11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A077KT11
B	-17	SER	-	expression tag	UNP A0A077KT11
B	-16	SER	-	expression tag	UNP A0A077KT11
B	-15	HIS	-	expression tag	UNP A0A077KT11
B	-14	HIS	-	expression tag	UNP A0A077KT11
B	-13	HIS	-	expression tag	UNP A0A077KT11
B	-12	HIS	-	expression tag	UNP A0A077KT11
B	-11	HIS	-	expression tag	UNP A0A077KT11
B	-10	HIS	-	expression tag	UNP A0A077KT11
B	-9	SER	-	expression tag	UNP A0A077KT11
B	-8	SER	-	expression tag	UNP A0A077KT11
B	-7	GLY	-	expression tag	UNP A0A077KT11
B	-6	LEU	-	expression tag	UNP A0A077KT11
B	-5	VAL	-	expression tag	UNP A0A077KT11
B	-4	PRO	-	expression tag	UNP A0A077KT11
B	-3	ARG	-	expression tag	UNP A0A077KT11
B	-2	GLY	-	expression tag	UNP A0A077KT11
B	-1	SER	-	expression tag	UNP A0A077KT11
B	0	HIS	-	expression tag	UNP A0A077KT11
C	-19	MET	-	initiating methionine	UNP A0A077KT11
C	-18	GLY	-	expression tag	UNP A0A077KT11
C	-17	SER	-	expression tag	UNP A0A077KT11
C	-16	SER	-	expression tag	UNP A0A077KT11
C	-15	HIS	-	expression tag	UNP A0A077KT11
C	-14	HIS	-	expression tag	UNP A0A077KT11
C	-13	HIS	-	expression tag	UNP A0A077KT11
C	-12	HIS	-	expression tag	UNP A0A077KT11
C	-11	HIS	-	expression tag	UNP A0A077KT11
C	-10	HIS	-	expression tag	UNP A0A077KT11
C	-9	SER	-	expression tag	UNP A0A077KT11
C	-8	SER	-	expression tag	UNP A0A077KT11
C	-7	GLY	-	expression tag	UNP A0A077KT11
C	-6	LEU	-	expression tag	UNP A0A077KT11
C	-5	VAL	-	expression tag	UNP A0A077KT11
C	-4	PRO	-	expression tag	UNP A0A077KT11
C	-3	ARG	-	expression tag	UNP A0A077KT11
C	-2	GLY	-	expression tag	UNP A0A077KT11
C	-1	SER	-	expression tag	UNP A0A077KT11
C	0	HIS	-	expression tag	UNP A0A077KT11
D	-19	MET	-	initiating methionine	UNP A0A077KT11
D	-18	GLY	-	expression tag	UNP A0A077KT11
D	-17	SER	-	expression tag	UNP A0A077KT11

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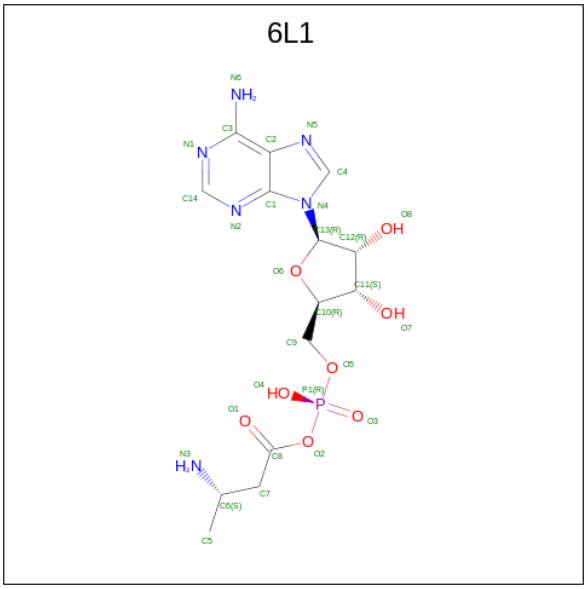
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A077KT11
D	-15	HIS	-	expression tag	UNP A0A077KT11
D	-14	HIS	-	expression tag	UNP A0A077KT11
D	-13	HIS	-	expression tag	UNP A0A077KT11
D	-12	HIS	-	expression tag	UNP A0A077KT11
D	-11	HIS	-	expression tag	UNP A0A077KT11
D	-10	HIS	-	expression tag	UNP A0A077KT11
D	-9	SER	-	expression tag	UNP A0A077KT11
D	-8	SER	-	expression tag	UNP A0A077KT11
D	-7	GLY	-	expression tag	UNP A0A077KT11
D	-6	LEU	-	expression tag	UNP A0A077KT11
D	-5	VAL	-	expression tag	UNP A0A077KT11
D	-4	PRO	-	expression tag	UNP A0A077KT11
D	-3	ARG	-	expression tag	UNP A0A077KT11
D	-2	GLY	-	expression tag	UNP A0A077KT11
D	-1	SER	-	expression tag	UNP A0A077KT11
D	0	HIS	-	expression tag	UNP A0A077KT11

- Molecule 2 is 5'-O-[(R)-{[(3S)-3-aminobutanoyl]oxy}(hydroxy)phosphoryl]adenosine (three-letter code: 6L1) (formula: $C_{14}H_{21}N_6O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	14	6	8	1		
2	B	1	Total	C	N	O	P	0	0
			29	14	6	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			29	14	6	8	1		
2	D	1	Total	C	N	O	P	0	0
			29	14	6	8	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

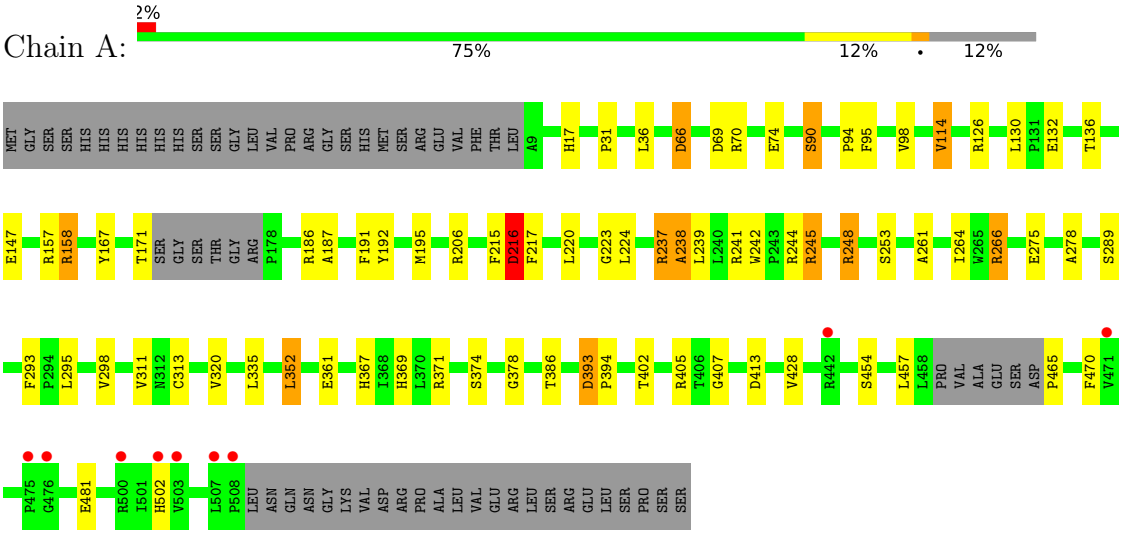
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	58	Total	O	0	0
			58	58		
4	C	69	Total	O	0	0
			69	69		
4	D	60	Total	O	0	0
			60	60		

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.

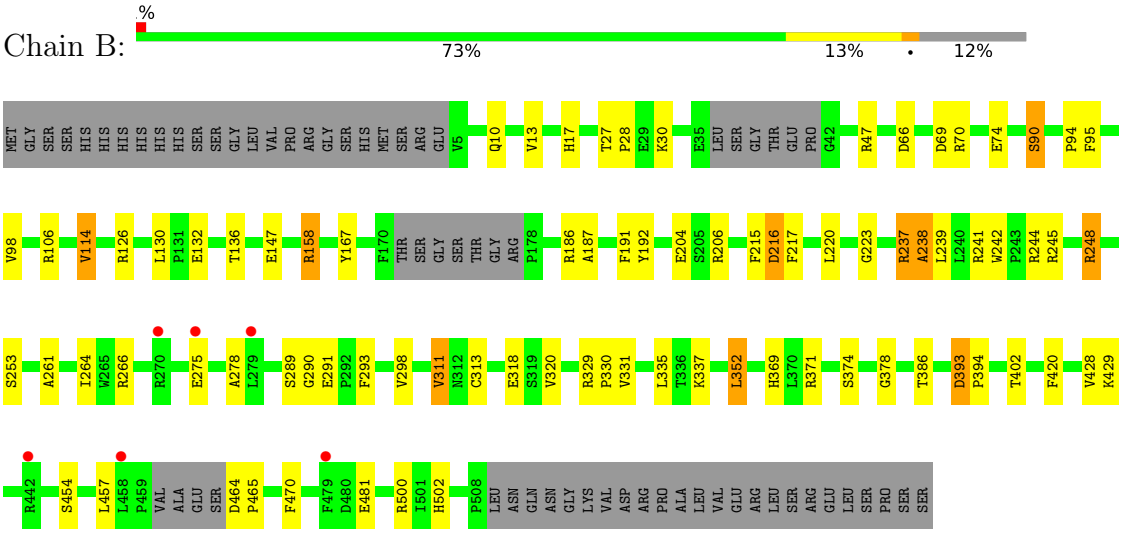
• Molecule 1: AMP-dependent synthetase and ligase

Chain A:



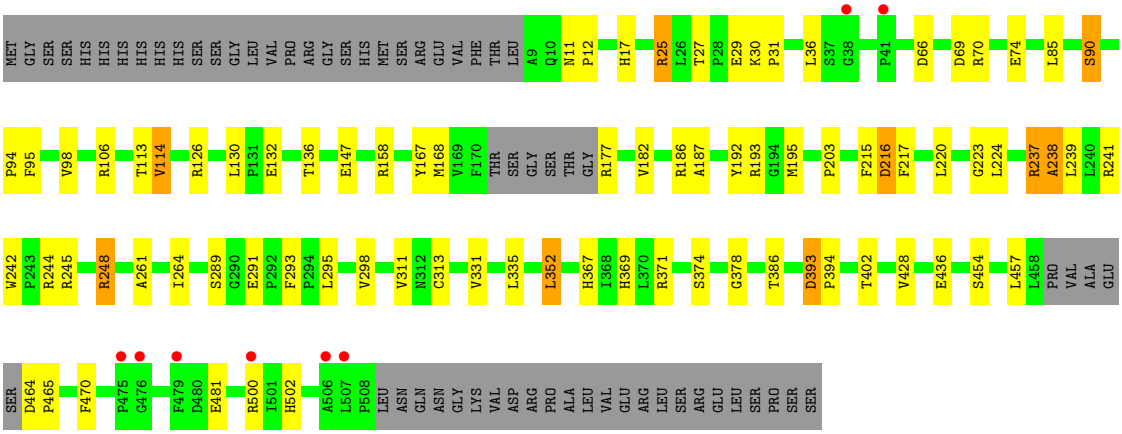
• Molecule 1: AMP-dependent synthetase and ligase

Chain B:



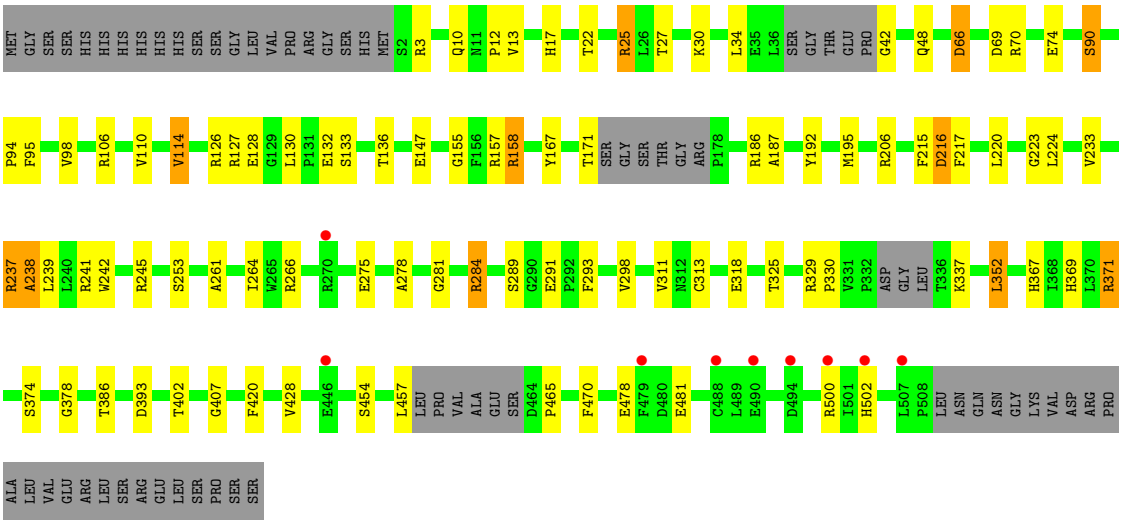
• Molecule 1: AMP-dependent synthetase and ligase

Chain C:



• Molecule 1: AMP-dependent synthetase and ligase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.75Å 104.45Å 120.00Å 81.78° 83.01° 81.98°	Depositor
Resolution (Å)	59.51 – 2.60 59.44 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (59.51-2.60) 94.1 (59.44-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.234 , 0.265 0.237 , 0.268	Depositor DCC
R_{free} test set	4516 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15125	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.69% 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: 6L1, CL

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	0.76	0/3770	0.87	7/5134 (0.1%)
1	B	0.68	0/3770	0.86	4/5134 (0.1%)
1	C	0.72	0/3782	0.87	4/5151 (0.1%)
1	D	0.70	0/3774	0.90	6/5136 (0.1%)
All	All	0.71	0/15096	0.87	21/20555 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	371	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	A	405	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	D	371	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	405	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	393	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	158	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	25	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	393	ASP	CB-CG-OD1	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	25	ARG	N-CA-CB	5.42	120.35	110.60
1	D	158	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	216	ASP	N-CA-CB	-5.26	101.13	110.60
1	D	25	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	393	ASP	CB-CG-OD1	5.23	123.00	118.30
1	C	393	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	266	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	158	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	393	ASP	CB-CG-OD1	5.20	122.97	118.30
1	B	216	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	413	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	266	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	266	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	PHE	Peptide
1	B	215	PHE	Peptide
1	C	215	PHE	Peptide
1	D	215	PHE	Peptide

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	3685	0	3677	36	0
1	B	3685	0	3676	42	0
1	C	3697	0	3685	39	0
1	D	3691	0	3681	46	0
2	A	29	0	0	2	0
2	B	29	0	0	3	0
2	C	29	0	0	1	0
2	D	29	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	60	0	0	1	0
4	B	58	0	0	1	0
4	C	69	0	0	1	0
4	D	60	0	0	1	0
All	All	15125	0	14719	152	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 5.

All (152) 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:D:281:GLY:O	1:D:284:ARG:NH1	2.04	0.91
1:A:206:ARG:NH2	1:C:25:ARG:O	2.21	0.72
1:D:127:ARG:O	1:D:128:GLU:HG3	1.99	0.63
1:C:30:LYS:NZ	1:C:203:PRO:O	2.31	0.62
1:C:69:ASP:O	1:C:94:PRO:HD2	2.00	0.61
1:A:69:ASP:O	1:A:94:PRO:HD2	2.01	0.60
1:D:289:SER:HB3	1:D:313:CYS:HB3	1.84	0.60
1:A:371:ARG:NH2	1:A:393:ASP:OD2	2.35	0.59
1:D:481:GLU:H	1:D:481:GLU:CD	2.05	0.59
1:B:47:ARG:HH22	1:D:48:GLN:HE22	1.50	0.59
1:A:289:SER:HB3	1:A:313:CYS:HB3	1.85	0.59
1:D:69:ASP:O	1:D:94:PRO:HD2	2.02	0.59
1:C:289:SER:HB3	1:C:313:CYS:HB3	1.84	0.59
1:B:371:ARG:NH2	1:B:393:ASP:OD2	2.37	0.58
1:D:187:ALA:HB1	1:D:374:SER:O	2.04	0.58
1:B:69:ASP:O	1:B:94:PRO:HD2	2.04	0.58
1:C:371:ARG:NH2	1:C:393:ASP:OD2	2.36	0.57
1:A:66:ASP:HA	4:A:736:HOH:O	2.04	0.57
1:C:187:ALA:HB1	1:C:374:SER:O	2.04	0.57
1:B:289:SER:HB3	1:B:313:CYS:HB3	1.86	0.57
1:B:187:ALA:HB1	1:B:374:SER:O	2.05	0.57
1:A:187:ALA:HB1	1:A:374:SER:O	2.04	0.56
1:B:27:THR:HB	1:B:30:LYS:HG2	1.88	0.56
1:A:186:ARG:O	1:A:187:ALA:C	2.41	0.56
1:D:186:ARG:O	1:D:187:ALA:C	2.43	0.56
1:B:28:PRO:HG2	1:D:48:GLN:HE21	1.70	0.55
1:D:367[B]:HIS:CD2	1:D:367[B]:HIS:C	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:O	1:B:187:ALA:C	2.43	0.54
1:D:192:TYR:CE1	1:D:223:GLY:HA3	2.43	0.54
1:A:241:ARG:O	1:A:242:TRP:CG	2.61	0.54
1:D:34:LEU:HD23	1:D:42:GLY:O	2.08	0.53
1:D:378:GLY:HA2	1:D:386:THR:HG23	1.91	0.53
2:A:601:6L1:N3	2:A:601:6L1:O2	2.41	0.53
1:C:378:GLY:HA2	1:C:386:THR:HG23	1.91	0.52
1:A:378:GLY:HA2	1:A:386:THR:HG23	1.92	0.52
1:B:378:GLY:HA2	1:B:386:THR:HG23	1.92	0.51
1:A:192:TYR:CE1	1:A:223:GLY:HA3	2.44	0.51
1:A:17:HIS:CE1	1:A:90:SER:HA	2.46	0.51
1:A:157:ARG:NH2	1:B:371:ARG:HD2	2.26	0.51
1:C:186:ARG:O	1:C:187:ALA:C	2.44	0.51
1:C:241:ARG:O	1:C:242:TRP:CG	2.64	0.50
1:B:17:HIS:CE1	1:B:90:SER:HA	2.47	0.50
1:B:241:ARG:O	1:B:242:TRP:CG	2.65	0.50
1:C:113:THR:HG22	1:C:177:ARG:NH2	2.27	0.50
1:C:192:TYR:CE1	1:C:223:GLY:HA3	2.47	0.50
1:D:17:HIS:CE1	1:D:90:SER:HA	2.46	0.50
1:C:136:THR:HG22	1:C:147:GLU:HB2	1.94	0.49
1:D:241:ARG:O	1:D:242:TRP:CG	2.65	0.49
1:B:47:ARG:NH2	1:D:48:GLN:HE22	2.11	0.49
1:A:136:THR:HG22	1:A:147:GLU:HB2	1.95	0.49
1:B:192:TYR:CE1	1:B:223:GLY:HA3	2.48	0.49
1:B:136:THR:HG22	1:B:147:GLU:HB2	1.95	0.49
1:C:95:PHE:CE2	1:C:167:TYR:HB3	2.48	0.48
1:B:70:ARG:HD2	1:B:114:VAL:HG22	1.95	0.48
1:D:70:ARG:HD2	1:D:114:VAL:HG22	1.96	0.48
1:B:244:ARG:O	1:B:248:ARG:HG2	2.14	0.48
1:D:242:TRP:HB3	1:D:245:ARG:HD2	1.96	0.47
1:C:244:ARG:O	1:C:248:ARG:HG2	2.14	0.47
1:C:295:LEU:HD13	1:C:335:LEU:O	2.14	0.47
1:A:95:PHE:CE2	1:A:167:TYR:HB3	2.49	0.47
1:A:244:ARG:O	1:A:248:ARG:HG2	2.14	0.47
1:B:28:PRO:CG	1:D:48:GLN:HE21	2.27	0.47
1:A:70:ARG:HD2	1:A:114:VAL:HG22	1.96	0.47
1:A:253:SER:HA	1:C:29:GLU:OE1	2.14	0.47
1:A:295:LEU:HD13	1:A:335:LEU:O	2.15	0.47
1:D:136:THR:HG22	1:D:147:GLU:HB2	1.95	0.47
1:D:457:LEU:HD21	1:D:465:PRO:HB2	1.96	0.47
1:B:457:LEU:HD21	1:B:465:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:HIS:CE1	1:C:90:SER:HA	2.51	0.46
1:B:290:GLY:HA2	2:B:601:6L1:O1	2.14	0.46
1:B:220:LEU:C	1:B:220:LEU:HD23	2.36	0.46
1:C:335:LEU:HA	4:C:706:HOH:O	2.14	0.46
1:D:261:ALA:O	1:D:264:ILE:HG12	2.14	0.46
1:A:367[B]:HIS:CE1	1:A:407:GLY:HA2	2.50	0.46
1:C:220:LEU:C	1:C:220:LEU:HD23	2.36	0.46
1:B:261:ALA:O	1:B:264:ILE:HG12	2.16	0.46
1:D:220:LEU:C	1:D:220:LEU:HD23	2.36	0.46
1:C:70:ARG:HD2	1:C:114:VAL:HG22	1.98	0.45
1:A:242:TRP:HB3	1:A:245:ARG:HD2	1.98	0.45
1:C:30:LYS:HG3	1:C:31:PRO:HD2	1.98	0.45
1:B:242:TRP:HB3	1:B:245:ARG:HD2	1.97	0.45
1:A:261:ALA:O	1:A:264:ILE:HG12	2.16	0.45
1:D:10:GLN:O	1:D:13:VAL:HG22	2.17	0.45
1:B:335:LEU:HA	1:B:335:LEU:HD12	1.67	0.45
1:C:187:ALA:HA	1:C:374:SER:HA	1.99	0.45
1:C:242:TRP:HB3	1:C:245:ARG:HD2	1.98	0.45
1:A:187:ALA:HA	1:A:374:SER:HA	1.99	0.45
1:C:261:ALA:O	1:C:264:ILE:HG12	2.17	0.45
1:C:457:LEU:HD21	1:C:465:PRO:HB2	1.98	0.45
1:B:393:ASP:HA	1:B:394:PRO:HD3	1.85	0.44
1:C:74:GLU:HA	1:C:98:VAL:O	2.17	0.44
1:A:216:ASP:OD2	2:A:601:6L1:N3	2.50	0.44
1:D:74:GLU:HA	1:D:98:VAL:O	2.18	0.44
1:D:34:LEU:HD12	1:D:233:VAL:HG22	1.98	0.44
1:B:95:PHE:CE2	1:B:167:TYR:HB3	2.52	0.44
1:A:220:LEU:C	1:A:220:LEU:HD23	2.38	0.44
1:D:352:LEU:HD22	1:D:369:HIS:CG	2.52	0.44
1:A:470:PHE:CD2	1:A:502:HIS:HB2	2.53	0.44
1:A:393:ASP:HA	1:A:394:PRO:HD3	1.86	0.44
1:A:457:LEU:HD21	1:A:465:PRO:HB2	2.00	0.44
1:B:320:VAL:O	2:B:601:6L1:N3	2.51	0.44
1:D:337:LYS:HE3	1:D:420:PHE:O	2.18	0.44
1:D:367[B]:HIS:CE1	1:D:407:GLY:HA2	2.53	0.44
1:B:10:GLN:O	1:B:13:VAL:HG22	2.17	0.43
1:C:367[B]:HIS:CD2	1:C:367[B]:HIS:C	2.91	0.43
1:C:393:ASP:HA	1:C:394:PRO:HD3	1.86	0.43
1:A:74:GLU:HA	1:A:98:VAL:O	2.18	0.43
1:B:352:LEU:HD22	1:B:369:HIS:CG	2.53	0.43
1:B:329:ARG:HA	1:B:330:PRO:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASP:OD2	2:C:601:6L1:N3	2.52	0.43
1:D:95:PHE:CE2	1:D:167:TYR:HB3	2.54	0.43
1:B:311:VAL:CG1	4:B:728:HOH:O	2.65	0.43
1:C:371:ARG:HD2	1:D:157:ARG:NH2	2.34	0.43
1:D:187:ALA:HA	1:D:374:SER:HA	2.01	0.43
1:A:70:ARG:HG2	1:A:94:PRO:HG2	2.01	0.43
1:A:266:ARG:HH11	1:A:266:ARG:HD2	1.65	0.43
1:B:47:ARG:HH22	1:D:48:GLN:NE2	2.16	0.43
1:D:206:ARG:NH1	1:D:253:SER:O	2.52	0.42
1:D:216:ASP:OD2	2:D:601:6L1:N3	2.52	0.42
1:D:237:ARG:O	1:D:238:ALA:C	2.57	0.42
1:A:237:ARG:O	1:A:238:ALA:C	2.57	0.42
1:B:275:GLU:O	1:B:278:ALA:HB3	2.20	0.42
1:B:337:LYS:HE3	1:B:420:PHE:O	2.19	0.42
1:C:470:PHE:CD2	1:C:502:HIS:HB2	2.54	0.42
1:D:66:ASP:OD2	1:D:155:GLY:N	2.52	0.42
1:D:275:GLU:O	1:D:278:ALA:HB3	2.19	0.42
1:A:352:LEU:HD22	1:A:369:HIS:CG	2.55	0.42
1:D:34:LEU:HD23	1:D:34:LEU:HA	1.86	0.42
1:A:31:PRO:HG3	1:C:27:THR:HG22	2.01	0.41
1:B:74:GLU:HA	1:B:98:VAL:O	2.19	0.41
1:C:352:LEU:HD22	1:C:369:HIS:CG	2.55	0.41
1:D:329:ARG:HA	1:D:330:PRO:HA	1.93	0.41
1:C:11:ASN:HA	1:C:12:PRO:HD2	1.99	0.41
1:B:47:ARG:NH2	1:D:48:GLN:NE2	2.68	0.41
1:B:331:VAL:HG13	1:B:335:LEU:HD23	2.01	0.41
1:B:237:ARG:O	1:B:238:ALA:C	2.58	0.41
1:B:470:PHE:CD2	1:B:502:HIS:HB2	2.55	0.41
1:C:331:VAL:HG13	1:C:335:LEU:HD23	2.02	0.41
1:A:275:GLU:O	1:A:278:ALA:HB3	2.21	0.41
1:D:325:THR:HG22	4:D:731:HOH:O	2.20	0.41
1:C:168:MET:HG2	1:C:182:VAL:HG22	2.03	0.41
1:C:193:ARG:NE	1:D:12:PRO:HA	2.36	0.41
1:D:470:PHE:CD2	1:D:502:HIS:HB2	2.56	0.41
1:C:237:ARG:O	1:C:238:ALA:C	2.59	0.41
1:D:27:THR:HB	1:D:30:LYS:CG	2.51	0.41
1:B:313:CYS:O	2:B:601:6L1:N6	2.54	0.40
1:A:191:PHE:CE2	1:A:320:VAL:HG11	2.56	0.40
1:B:206:ARG:NH1	1:B:253:SER:O	2.54	0.40
1:B:191:PHE:CE2	1:B:320:VAL:HG11	2.57	0.40
1:A:195:MET:SD	1:A:224:LEU:HD13	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:MET:SD	1:C:224:LEU:HD13	2.61	0.40
1:D:195:MET:SD	1:D:224:LEU:HD13	2.61	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	483/552 (88%)	457 (95%)	24 (5%)	2 (0%)	34	57
1	B	480/552 (87%)	452 (94%)	25 (5%)	3 (1%)	25	47
1	C	484/552 (88%)	456 (94%)	26 (5%)	2 (0%)	34	57
1	D	478/552 (87%)	451 (94%)	24 (5%)	3 (1%)	25	47
All	All	1925/2208 (87%)	1816 (94%)	99 (5%)	10 (0%)	29	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ASP
1	B	216	ASP
1	C	216	ASP
1	D	216	ASP
1	A	238	ALA
1	B	238	ALA
1	B	318	GLU
1	C	238	ALA
1	D	238	ALA
1	D	318	GLU

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	384/439 (88%)	361 (94%)	23 (6%)	19	39
1	B	384/439 (88%)	359 (94%)	25 (6%)	17	34
1	C	385/439 (88%)	359 (93%)	26 (7%)	16	32
1	D	385/439 (88%)	356 (92%)	29 (8%)	13	27
All	All	1538/1756 (88%)	1435 (93%)	103 (7%)	16	33

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	66	ASP
1	A	90	SER
1	A	114	VAL
1	A	126	ARG
1	A	130	LEU
1	A	132	GLU
1	A	158	ARG
1	A	171	THR
1	A	217	PHE
1	A	237	ARG
1	A	239	LEU
1	A	245	ARG
1	A	248	ARG
1	A	293	PHE
1	A	298	VAL
1	A	311	VAL
1	A	352	LEU
1	A	361	GLU
1	A	402	THR
1	A	428	VAL
1	A	454	SER
1	A	481	GLU
1	B	66	ASP

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Mol	Chain	Res	Type
1	B	90	SER
1	B	106	ARG
1	B	114	VAL
1	B	126	ARG
1	B	130	LEU
1	B	132	GLU
1	B	158	ARG
1	B	204	GLU
1	B	217	PHE
1	B	237	ARG
1	B	239	LEU
1	B	248	ARG
1	B	291	GLU
1	B	293	PHE
1	B	298	VAL
1	B	311	VAL
1	B	352	LEU
1	B	402	THR
1	B	428	VAL
1	B	429	LYS
1	B	454	SER
1	B	464	ASP
1	B	481	GLU
1	B	500	ARG
1	C	36	LEU
1	C	66	ASP
1	C	85	LEU
1	C	90	SER
1	C	106	ARG
1	C	114	VAL
1	C	126	ARG
1	C	130	LEU
1	C	132	GLU
1	C	158	ARG
1	C	217	PHE
1	C	237	ARG
1	C	239	LEU
1	C	248	ARG
1	C	291	GLU
1	C	293	PHE
1	C	298	VAL
1	C	311	VAL

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Mol	Chain	Res	Type
1	C	352	LEU
1	C	402	THR
1	C	428	VAL
1	C	436	GLU
1	C	454	SER
1	C	464	ASP
1	C	481	GLU
1	C	500	ARG
1	D	3	ARG
1	D	22	THR
1	D	25	ARG
1	D	66	ASP
1	D	90	SER
1	D	106	ARG
1	D	110	VAL
1	D	114	VAL
1	D	126	ARG
1	D	130	LEU
1	D	132	GLU
1	D	133	SER
1	D	158	ARG
1	D	171	THR
1	D	217	PHE
1	D	237	ARG
1	D	239	LEU
1	D	284	ARG
1	D	291	GLU
1	D	293	PHE
1	D	298	VAL
1	D	311	VAL
1	D	352	LEU
1	D	371	ARG
1	D	402	THR
1	D	428	VAL
1	D	454	SER
1	D	478	GLU
1	D	500	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 8 ligands modelled in this entry, 4 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	6L1	B	601	-	27,31,31	2.56	8 (29%)	29,46,46	1.91	8 (27%)
2	6L1	C	601	-	27,31,31	2.27	7 (25%)	29,46,46	1.75	6 (20%)
2	6L1	A	601	-	27,31,31	2.44	9 (33%)	29,46,46	1.89	6 (20%)
2	6L1	D	601	-	27,31,31	2.52	8 (29%)	29,46,46	2.41	11 (37%)

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	6L1	B	601	-	-	4/13/35/35	0/3/3/3
2	6L1	C	601	-	-	3/13/35/35	0/3/3/3
2	6L1	A	601	-	-	8/13/35/35	0/3/3/3
2	6L1	D	601	-	-	5/13/35/35	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	6L1	C12-C13	-7.67	1.42	1.53
2	C	601	6L1	C14-N1	6.56	1.46	1.33
2	B	601	6L1	C14-N1	6.28	1.45	1.33
2	B	601	6L1	C14-N2	6.18	1.42	1.32
2	B	601	6L1	O6-C13	5.79	1.49	1.41
2	A	601	6L1	C12-C13	-5.72	1.45	1.53
2	D	601	6L1	C14-N2	5.62	1.41	1.32
2	A	601	6L1	O6-C13	5.49	1.48	1.41
2	C	601	6L1	O6-C13	5.08	1.48	1.41
2	A	601	6L1	C14-N1	5.01	1.43	1.33
2	C	601	6L1	P1-O2	4.39	1.69	1.60
2	D	601	6L1	O6-C13	4.05	1.46	1.41
2	B	601	6L1	P1-O2	3.88	1.68	1.60
2	B	601	6L1	C12-C13	-3.54	1.48	1.53
2	D	601	6L1	C14-N1	3.54	1.40	1.33
2	A	601	6L1	C14-N2	3.54	1.37	1.32
2	D	601	6L1	O8-C12	-3.51	1.34	1.43
2	A	601	6L1	P1-O3	3.48	1.63	1.50
2	C	601	6L1	C14-N2	3.36	1.37	1.32
2	D	601	6L1	P1-O3	3.13	1.62	1.50
2	B	601	6L1	C7-C8	2.96	1.56	1.50
2	C	601	6L1	O8-C12	2.76	1.49	1.43
2	A	601	6L1	C7-C6	-2.49	1.49	1.53
2	A	601	6L1	C7-C8	2.48	1.55	1.50
2	D	601	6L1	C11-C10	-2.45	1.46	1.53
2	B	601	6L1	C2-C1	-2.43	1.34	1.40
2	B	601	6L1	C3-C2	-2.27	1.34	1.43
2	C	601	6L1	C7-C8	2.20	1.55	1.50
2	D	601	6L1	C7-C8	2.19	1.55	1.50
2	A	601	6L1	C3-C2	-2.19	1.35	1.43
2	C	601	6L1	C3-C2	-2.14	1.35	1.43
2	A	601	6L1	P1-O5	2.06	1.67	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	6L1	N2-C14-N1	-6.96	117.80	128.68
2	A	601	6L1	N2-C14-N1	-6.68	118.24	128.68
2	C	601	6L1	N2-C14-N1	-5.72	119.73	128.68
2	B	601	6L1	N2-C14-N1	-4.80	121.18	128.68
2	D	601	6L1	C13-N4-C1	-4.45	118.82	126.64
2	D	601	6L1	O6-C13-C12	-4.21	100.78	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	6L1	O2-P1-O5	4.18	115.14	102.92
2	D	601	6L1	O4-P1-O2	3.68	116.17	104.14
2	A	601	6L1	C13-N4-C1	-3.59	120.33	126.64
2	A	601	6L1	O6-C10-C9	3.30	120.22	109.37
2	B	601	6L1	C14-N1-C3	-3.19	113.30	118.75
2	D	601	6L1	O1-C8-C7	-3.06	117.97	124.73
2	D	601	6L1	O6-C10-C9	-2.98	99.58	109.37
2	D	601	6L1	O2-P1-O5	2.96	111.58	102.92
2	B	601	6L1	C2-C3-N6	-2.85	116.01	120.35
2	D	601	6L1	O5-P1-O3	-2.78	98.22	109.07
2	A	601	6L1	O2-C8-C7	2.74	118.65	111.11
2	C	601	6L1	O6-C10-C9	2.69	118.23	109.37
2	B	601	6L1	O2-C8-C7	2.66	118.43	111.11
2	C	601	6L1	C5-C6-C7	2.47	114.80	111.94
2	C	601	6L1	C13-N4-C1	-2.47	122.30	126.64
2	C	601	6L1	O2-P1-O5	2.36	109.81	102.92
2	A	601	6L1	O8-C12-C11	-2.33	104.28	111.82
2	C	601	6L1	O2-C8-C7	2.28	117.37	111.11
2	A	601	6L1	O4-P1-O5	2.26	118.25	107.75
2	D	601	6L1	O2-C8-C7	2.26	117.33	111.11
2	D	601	6L1	O2-P1-O3	-2.22	102.60	109.45
2	B	601	6L1	C13-N4-C1	2.14	130.40	126.64
2	B	601	6L1	C2-C3-N1	2.13	125.18	120.35
2	B	601	6L1	O1-C8-C7	-2.06	120.19	124.73
2	D	601	6L1	C1-C2-N5	-2.00	107.31	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	6L1	C9-O5-P1-O3
2	A	601	6L1	C9-O5-P1-O4
2	A	601	6L1	O6-C10-C9-O5
2	A	601	6L1	C11-C10-C9-O5
2	D	601	6L1	C9-O5-P1-O3
2	D	601	6L1	C9-O5-P1-O4
2	D	601	6L1	C11-C10-C9-O5
2	C	601	6L1	C11-C10-C9-O5
2	D	601	6L1	O6-C10-C9-O5
2	C	601	6L1	O6-C10-C9-O5
2	A	601	6L1	C9-O5-P1-O2
2	D	601	6L1	C9-O5-P1-O2

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Mol	Chain	Res	Type	Atoms
2	A	601	6L1	C8-O2-P1-O5
2	B	601	6L1	C8-O2-P1-O3
2	B	601	6L1	C8-O2-P1-O5
2	C	601	6L1	C8-O2-P1-O5
2	A	601	6L1	C6-C7-C8-O2
2	B	601	6L1	C6-C7-C8-O2
2	B	601	6L1	C6-C7-C8-O1
2	A	601	6L1	C6-C7-C8-O1

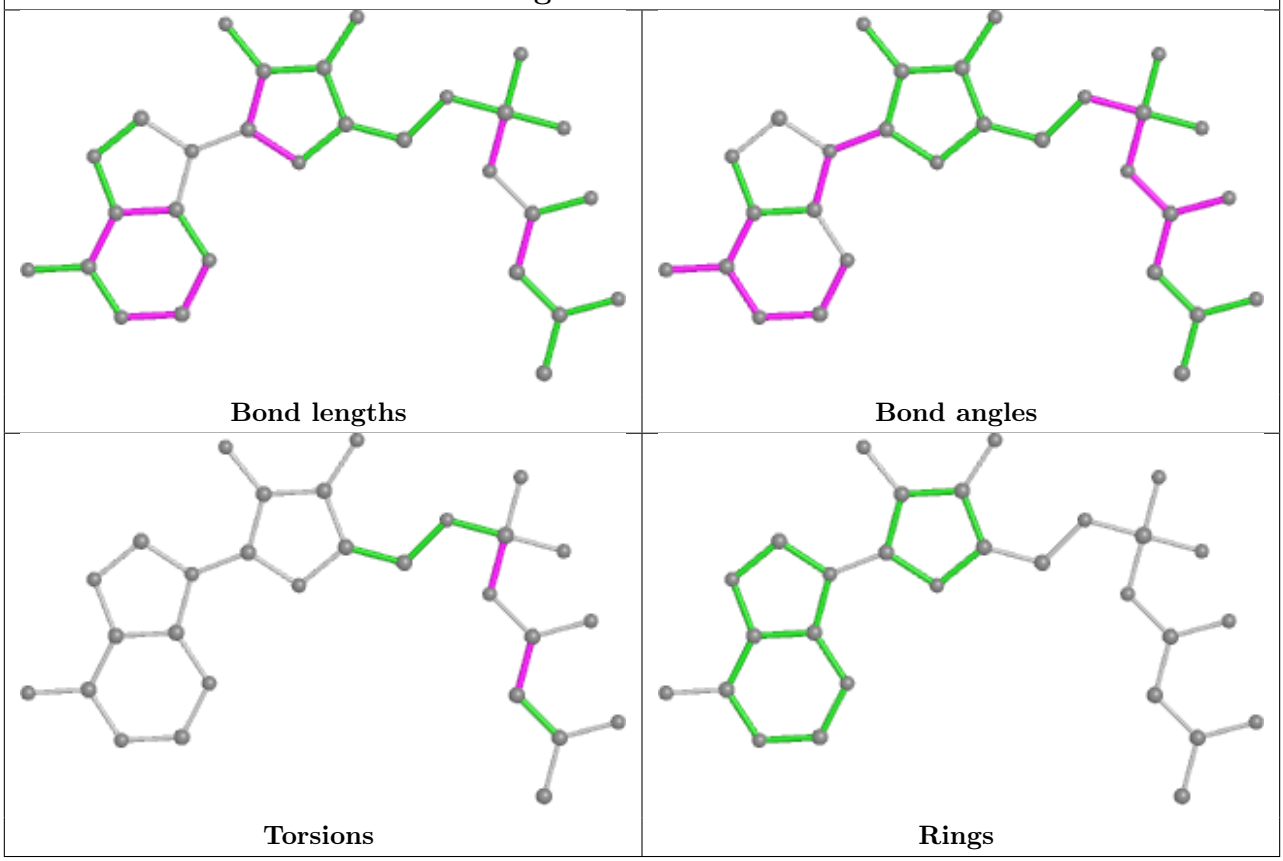
There are no ring outliers.

4 monomers are involved in 7 short contacts:

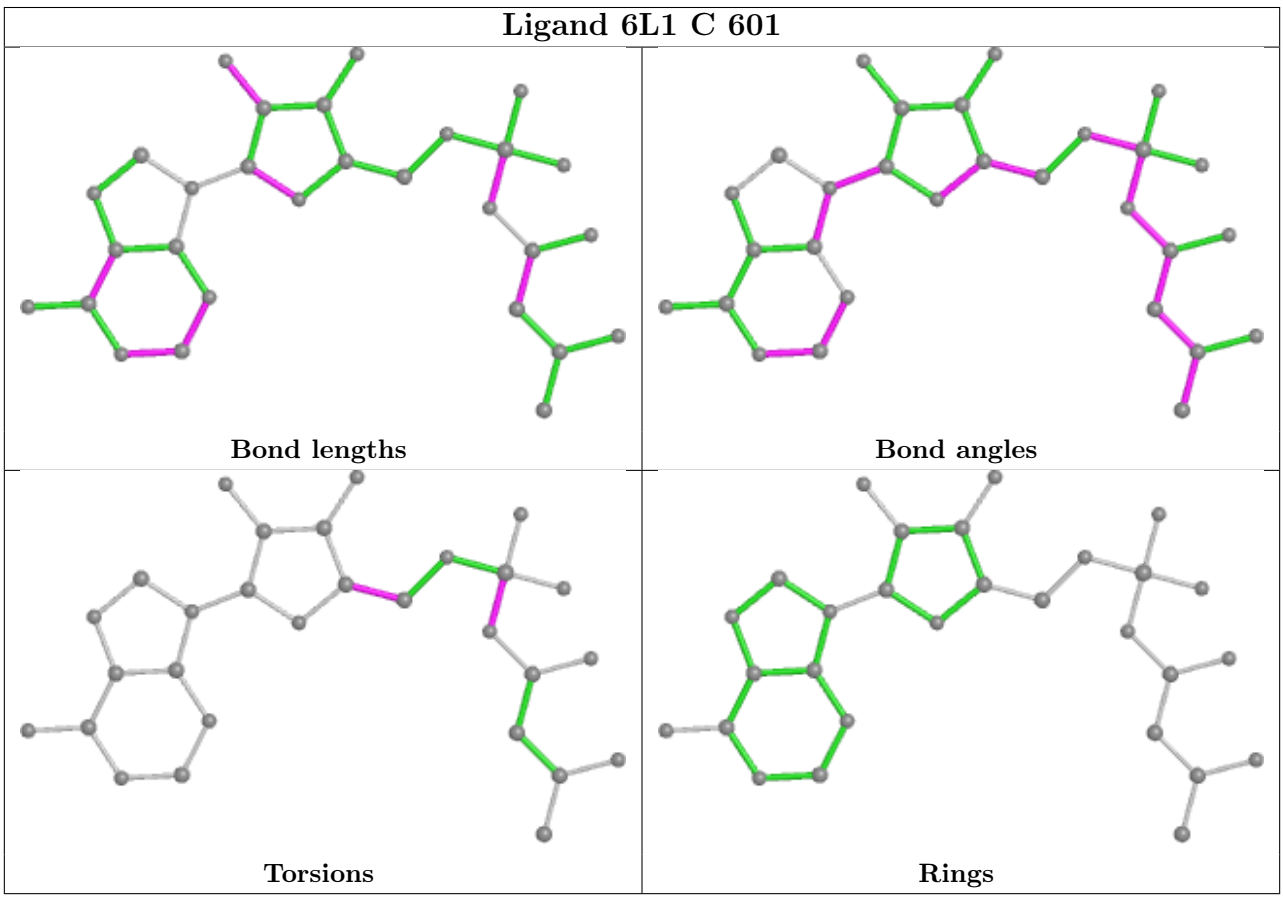
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	6L1	3	0
2	C	601	6L1	1	0
2	A	601	6L1	2	0
2	D	601	6L1	1	0

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.

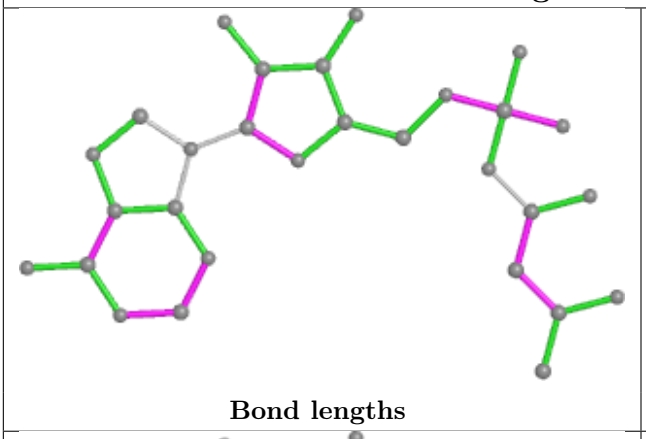
Ligand 6L1 B 601



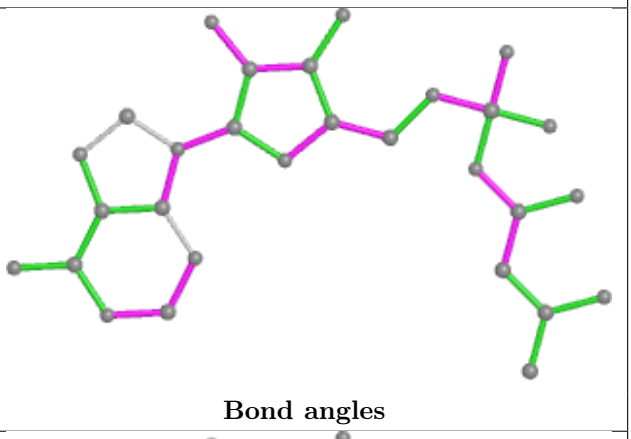
Ligand 6L1 C 601



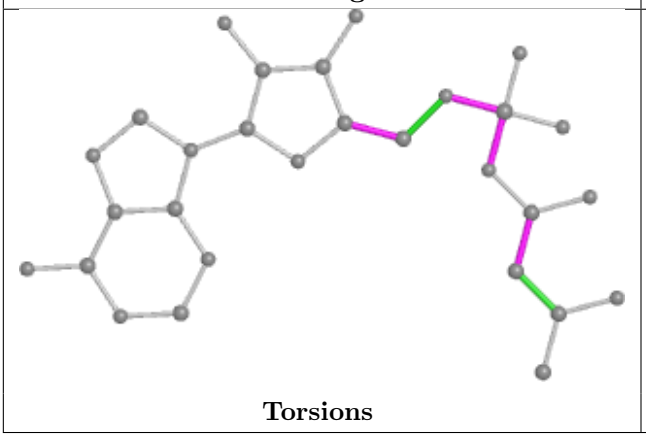
Ligand 6L1 A 601



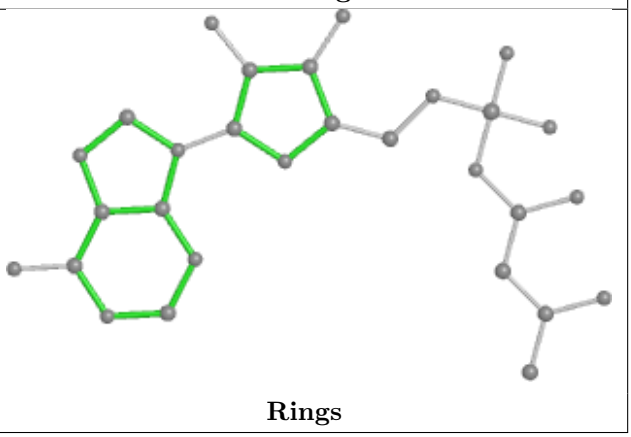
Bond lengths



Bond angles

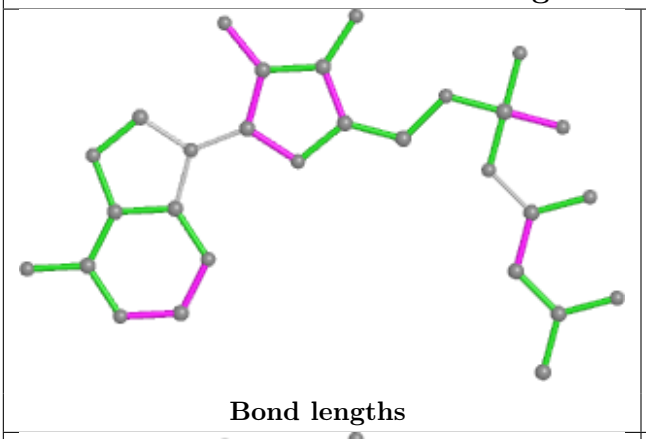


Torsions

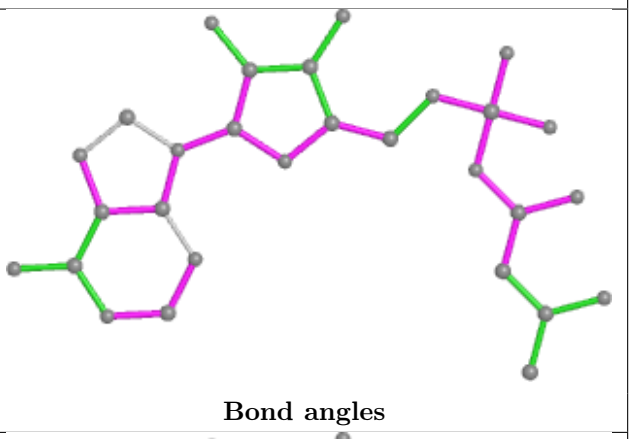


Rings

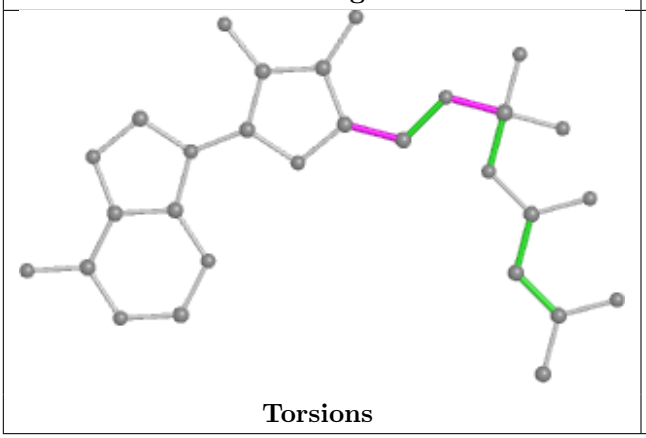
Ligand 6L1 D 601



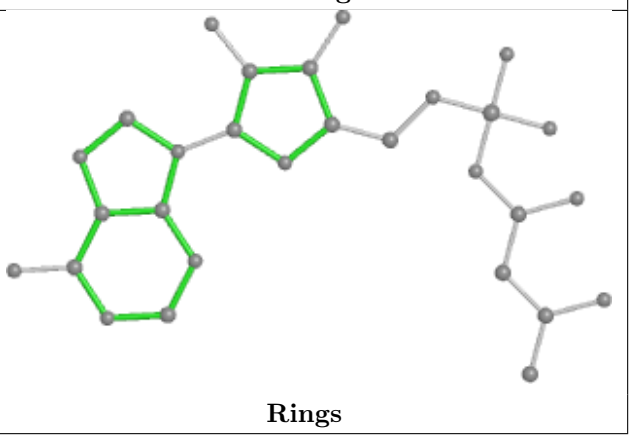
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	488/552 (88%)	-0.14	9 (1%)	68	64	15, 36, 71, 100	0
1	B	487/552 (88%)	-0.10	6 (1%)	79	76	16, 41, 83, 102	0
1	C	489/552 (88%)	-0.13	8 (1%)	72	68	17, 37, 78, 94	0
1	D	487/552 (88%)	-0.08	9 (1%)	68	64	16, 40, 80, 112	0
All	All	1951/2208 (88%)	-0.11	32 (1%)	72	68	15, 39, 79, 112	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	476	GLY	4.2
1	D	488	CYS	3.8
1	D	490	GLU	3.6
1	B	279	LEU	3.2
1	A	507	LEU	3.1
1	B	458	LEU	3.1
1	C	507	LEU	3.0
1	C	475	PRO	3.0
1	C	38	GLY	2.9
1	A	475	PRO	2.9
1	C	506	ALA	2.7
1	D	270	ARG	2.7
1	A	442	ARG	2.6
1	C	479	PHE	2.6
1	D	479	PHE	2.5
1	D	507	LEU	2.5
1	A	500	ARG	2.5
1	D	502	HIS	2.4
1	B	479	PHE	2.4
1	C	41	PRO	2.4
1	B	442	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	503	VAL	2.3
1	A	476	GLY	2.3
1	A	471	VAL	2.3
1	B	270	ARG	2.3
1	D	446	GLU	2.3
1	D	494	ASP	2.3
1	D	500	ARG	2.2
1	C	500	ARG	2.2
1	B	275	GLU	2.1
1	A	502	HIS	2.1
1	A	508	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

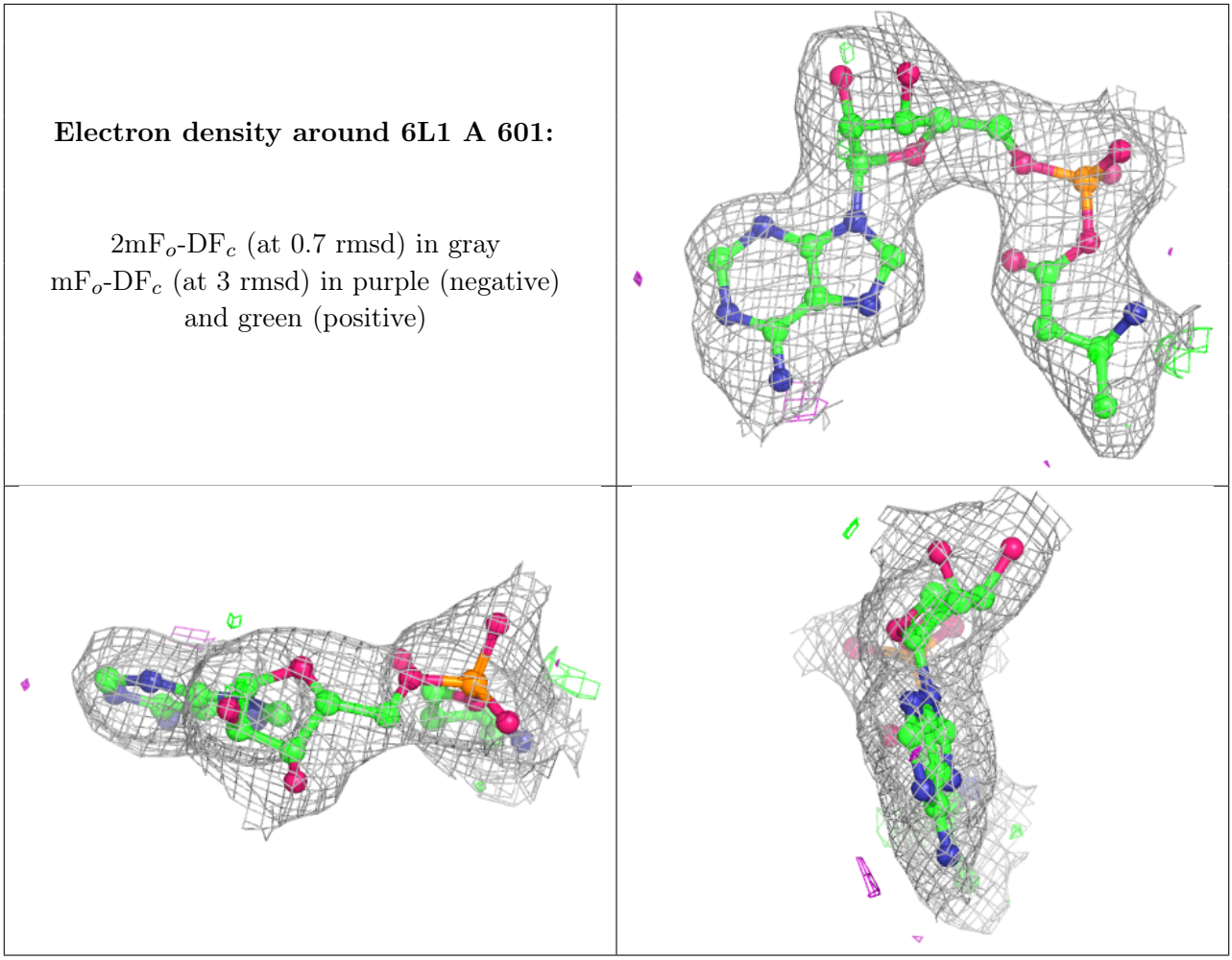
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	6L1	A	601	29/29	0.97	0.13	20,31,39,48	0
2	6L1	B	601	29/29	0.97	0.13	22,29,35,42	0
2	6L1	C	601	29/29	0.97	0.12	21,28,37,47	0
2	6L1	D	601	29/29	0.97	0.13	23,34,42,44	0
3	CL	B	602	1/1	0.98	0.07	30,30,30,30	0
3	CL	C	602	1/1	0.98	0.05	24,24,24,24	0
3	CL	D	602	1/1	0.98	0.10	33,33,33,33	0
3	CL	A	602	1/1	0.99	0.09	34,34,34,34	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.

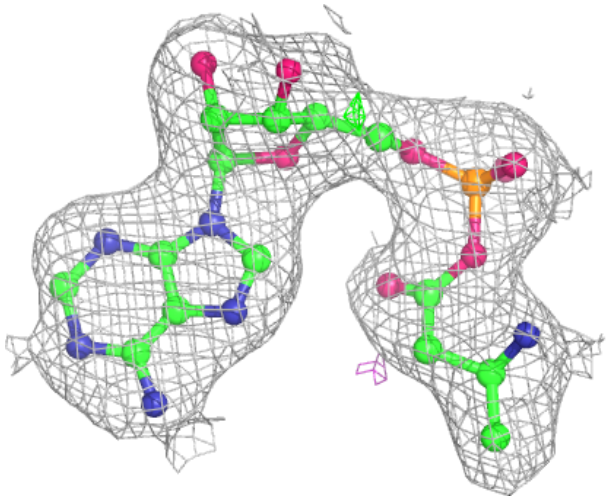
Electron density around 6L1 A 601:

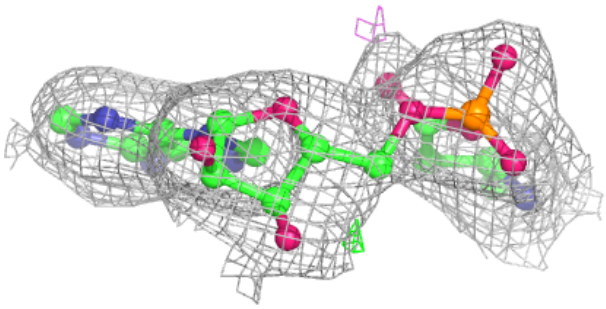
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

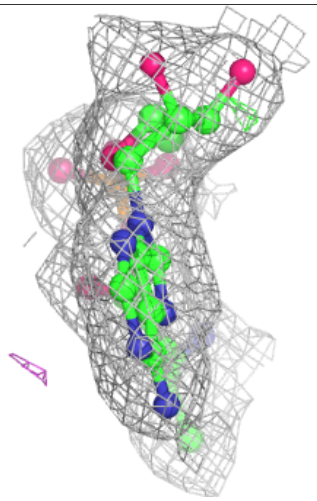


Electron density around 6L1 B 601:

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

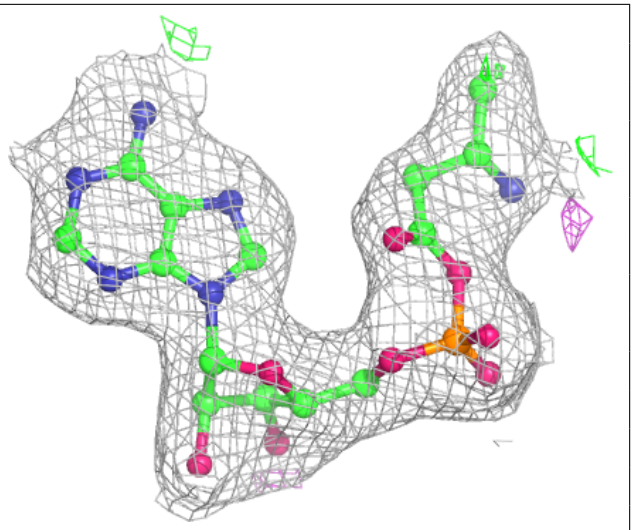


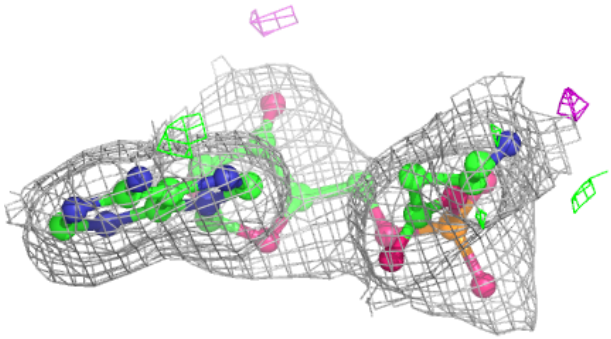


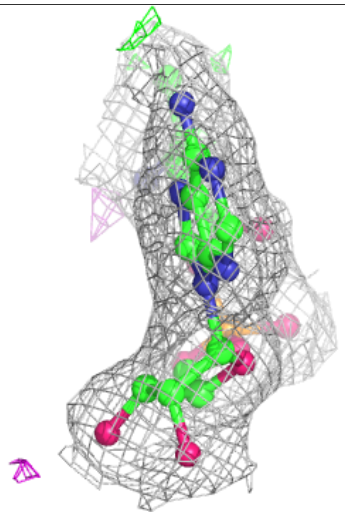


Electron density around 6L1 C 601:

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

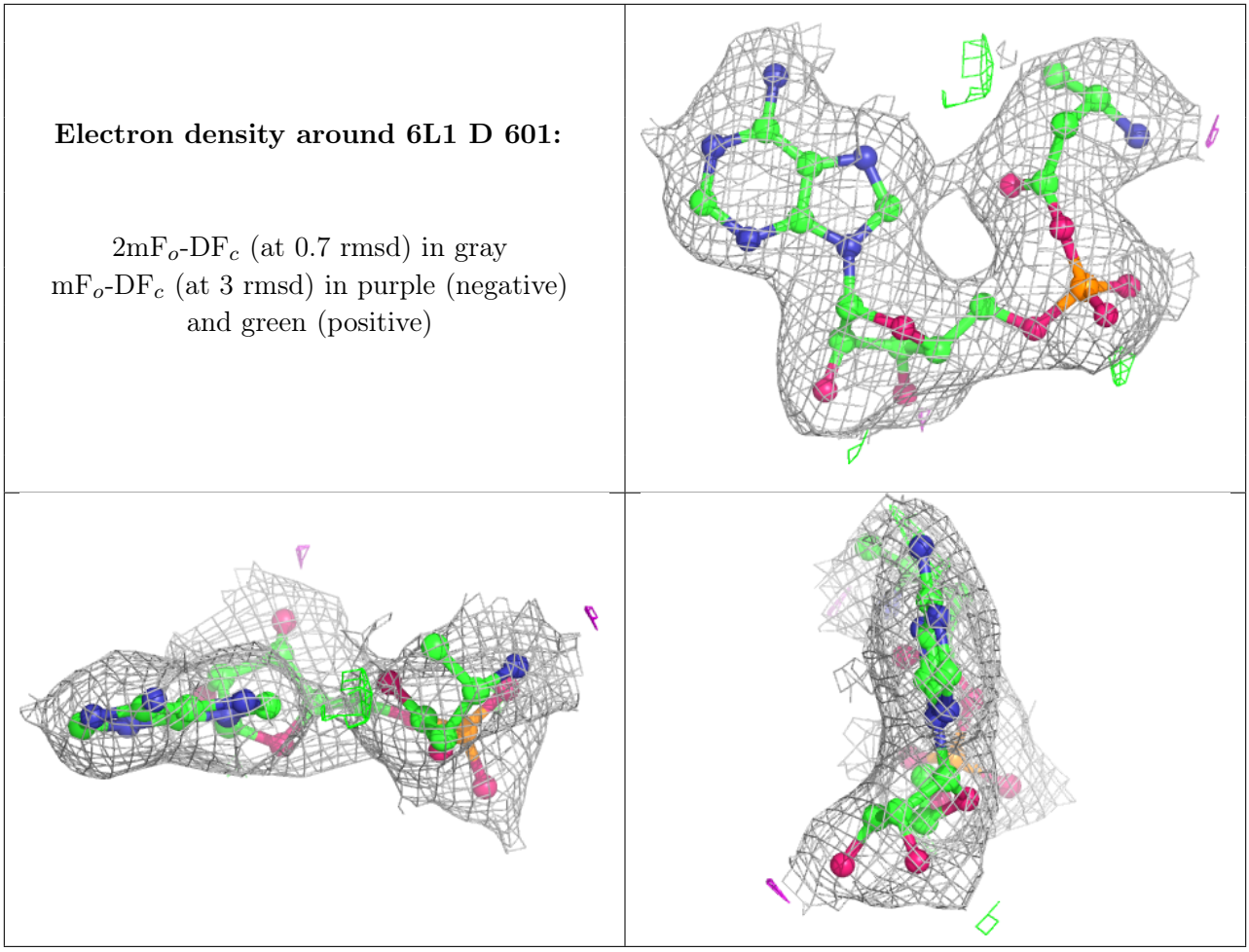






Electron density around 6L1 D 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.