



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 12:06 am BST

PDB ID : 6HCU  
Title : Crystal Structure of Lysyl-tRNA Synthetase from Plasmodium falciparum bound to a difluoro cyclohexyl chromone ligand  
Authors : Tamjar, J.; Robinson, D.A.; Baragana, B.; Norcross, N.; Forte, B.; Walpole, C.; Gilbert, I.H.  
Deposited on : 2018-08-16  
Resolution : 1.62 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

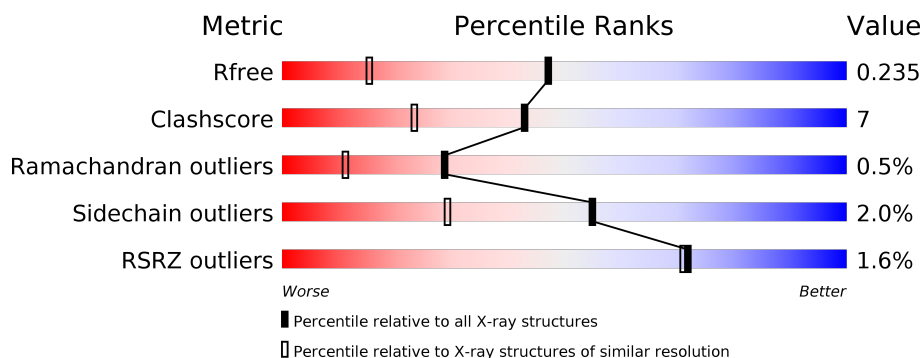
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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 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	507	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>• •</div> </div> </div>
1	B	507	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HIS	A	604	-	-	X	-
6	TRS	A	605	-	X	-	-
6	TRS	B	603	-	X	-	-

## 2 Entry composition [i](#)

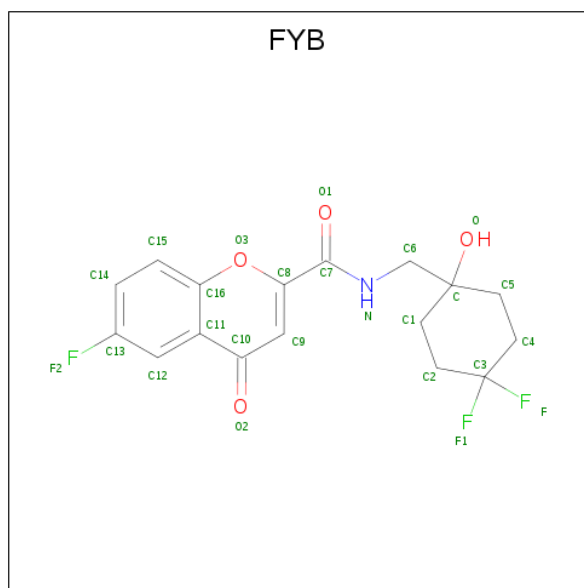
There are 7 unique types of molecules in this entry. The entry contains 9037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine-tRNA ligase.

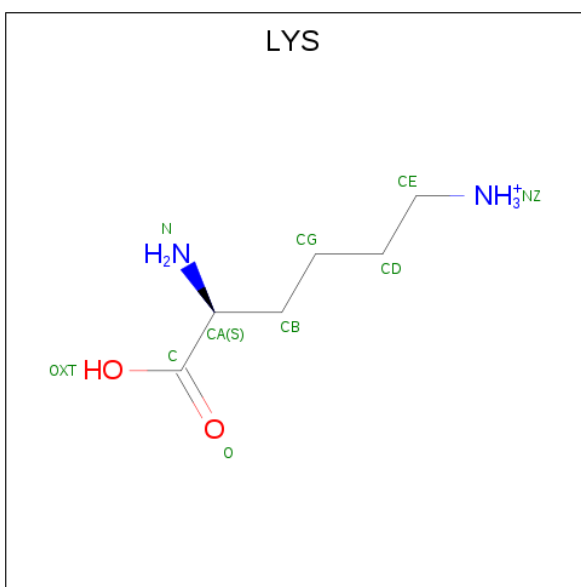
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	13	0
			4015	2598	663	731	23			
1	B	485	Total	C	N	O	S	0	9	0
			3949	2558	652	719	20			

- Molecule 2 is {N}-[[4,4-bis(fluoranyl)-1-oxidanyl-cyclohexyl]methyl]-6-fluoranyl-4-oxidanylidene-chromene-2-carboxamide (three-letter code: FYB) (formula: C<sub>17</sub>H<sub>16</sub>F<sub>3</sub>NO<sub>4</sub>).



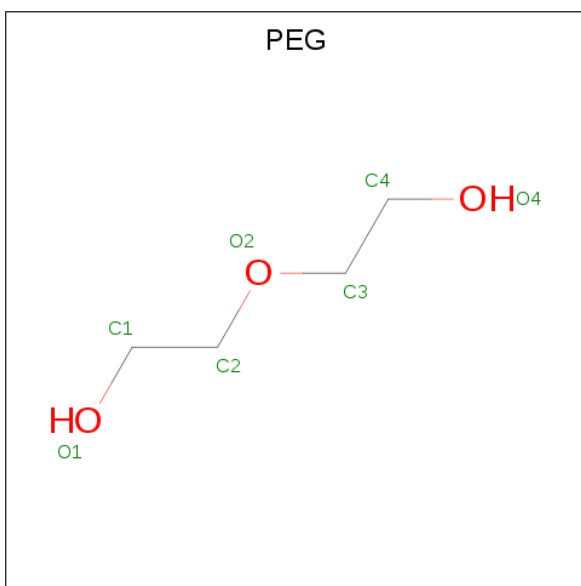
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			25	17	3	1	4		
2	B	1	Total	C	F	N	O	0	0
			25	17	3	1	4		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>).



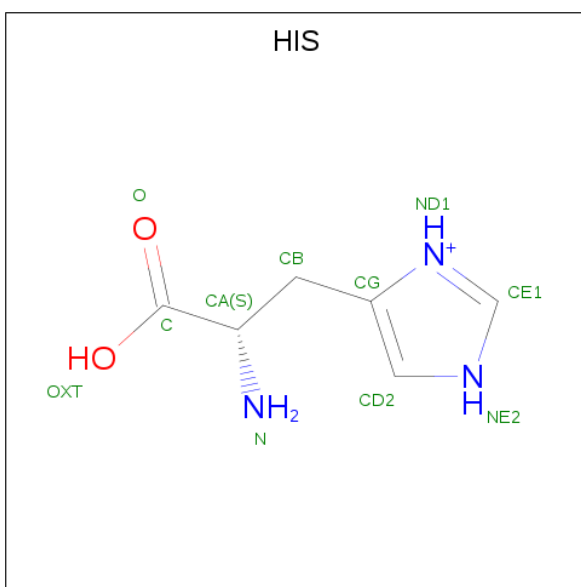
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



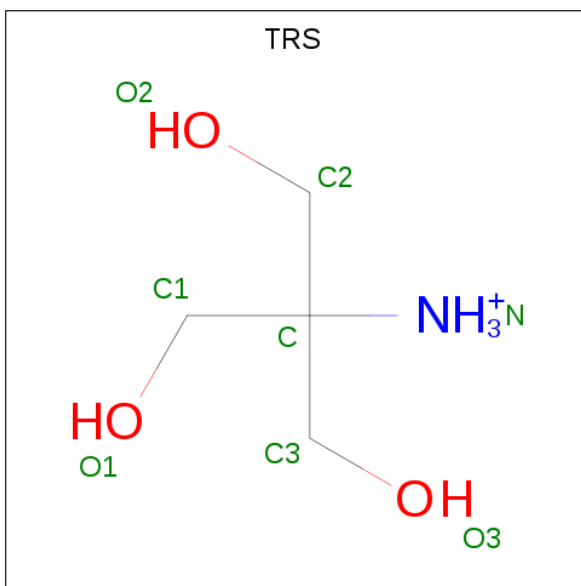
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is HISTIDINE (three-letter code: HIS) (formula: C<sub>6</sub>H<sub>10</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

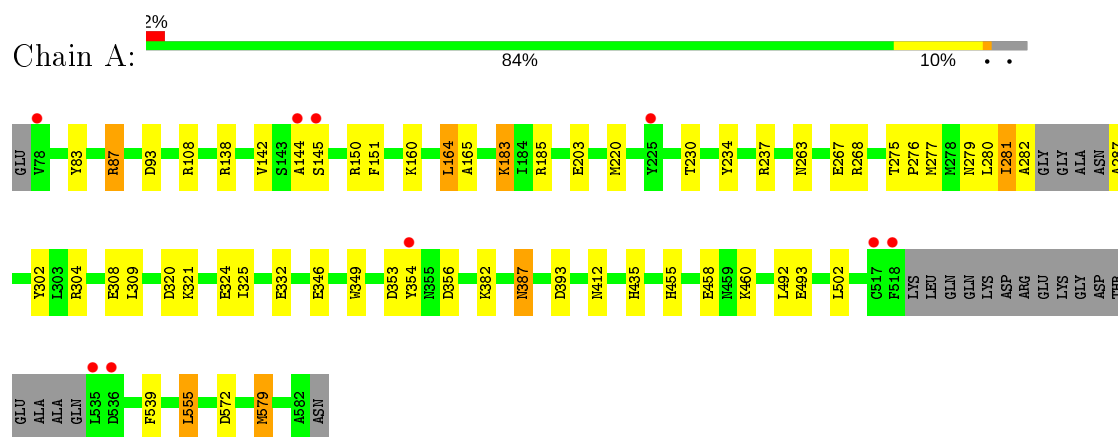
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	515	Total	O	0	0
			515	515		
7	B	451	Total	O	0	0
			451	451		

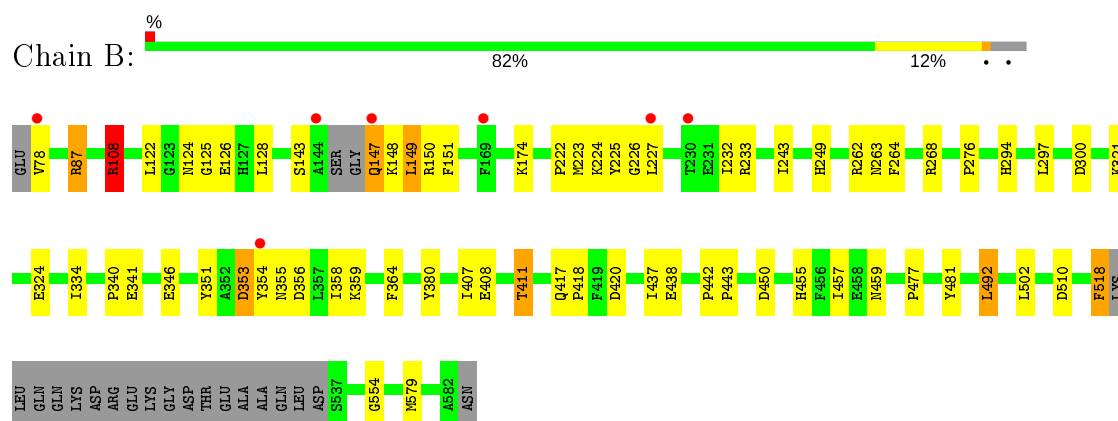
### 3 Residue-property plots [i](#)

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: Lysine-tRNA ligase



#### • Molecule 1: Lysine-tRNA ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.14Å 95.34Å 166.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.74 – 1.62 62.71 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.3 (82.74-1.62) 99.3 (62.71-1.62)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.183 , 0.226 0.194 , 0.235	Depositor DCC
$R_{free}$ test set	7280 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FYB, TRS, PEG

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	1.19	6/4155 (0.1%)	1.17	20/5612 (0.4%)
1	B	1.14	6/4073 (0.1%)	1.16	20/5508 (0.4%)
All	All	1.17	12/8228 (0.1%)	1.16	40/11120 (0.4%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	ASP	CB-CG	6.17	1.64	1.51
1	A	346	GLU	CG-CD	5.96	1.60	1.51
1	A	354	TYR	CE1-CZ	5.90	1.46	1.38
1	B	380	TYR	CE1-CZ	-5.69	1.31	1.38
1	B	346	GLU	CD-OE1	-5.52	1.19	1.25
1	B	341	GLU	CD-OE1	-5.50	1.19	1.25
1	A	108	ARG	CZ-NH1	-5.31	1.26	1.33
1	B	268	ARG	CZ-NH1	5.25	1.39	1.33
1	B	380	TYR	CG-CD2	-5.25	1.32	1.39
1	A	203	GLU	CD-OE1	5.24	1.31	1.25
1	A	458	GLU	CD-OE2	5.17	1.31	1.25
1	A	324	GLU	CD-OE1	-5.01	1.20	1.25

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ARG	NE-CZ-NH1	14.33	127.46	120.30
1	B	87	ARG	NE-CZ-NH2	-13.73	113.43	120.30
1	A	87	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	B	87	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	B	353	ASP	CB-CG-OD1	8.63	126.07	118.30
1	B	108	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	268	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	268	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	555	LEU	CB-CG-CD2	-7.12	98.89	111.00
1	B	300	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	185	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	268	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	579	MET	CA-CB-CG	6.59	124.50	113.30
1	B	324	GLU	OE1-CD-OE2	6.27	130.82	123.30
1	A	183	LYS	CB-CA-C	-6.26	97.87	110.40
1	B	264	PHE	CB-CG-CD1	6.22	125.16	120.80
1	B	300	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	237	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	B	579	MET	CA-CB-CG	6.08	123.64	113.30
1	A	353	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	320	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	A	281	ILE	N-CA-C	-6.00	94.80	111.00
1	A	356	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	A	393	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	481	TYR	CB-CG-CD1	5.78	124.47	121.00
1	B	262	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	510	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	138	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	164	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	B	420	ASP	CB-CG-OD1	5.38	123.15	118.30
1	B	150	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	364	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	B	353	ASP	OD1-CG-OD2	-5.28	113.28	123.30
1	B	233	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	572	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	481	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	B	108	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	579	MET	CG-SD-CE	5.11	108.37	100.20
1	A	493	GLU	N-CA-CB	-5.10	101.42	110.60
1	A	324	GLU	OE1-CD-OE2	5.07	129.38	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ALA	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	4015	0	4020	53	0
1	B	3949	0	3908	47	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
3	A	8	0	5	5	0
4	A	7	0	10	3	0
5	A	10	0	6	16	0
6	A	16	0	23	4	0
6	B	16	0	24	3	0
7	A	515	0	0	21	1
7	B	451	0	0	21	1
All	All	9037	0	7996	109	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 7.

All (109) 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:B:353:ASP:HB2	7:B:831:HOH:O	1.50	1.10
1:B:353:ASP:CB	7:B:831:HOH:O	2.00	1.05
6:B:602:TRS:O3	7:B:701:HOH:O	1.89	0.90
1:A:455:HIS:NE2	5:A:604:HIS:CD2	2.44	0.86
1:A:435:HIS:HD1	5:A:604:HIS:CE1	1.94	0.84
1:A:321[A]:LYS:HE3	3:A:602:LYS:HG3	1.58	0.84
1:A:455:HIS:NE2	5:A:604:HIS:CE1	2.46	0.83
1:B:321[B]:LYS:NZ	7:B:702:HOH:O	2.08	0.83
1:B:263[A]:ASN:ND2	7:B:703:HOH:O	2.17	0.76
1:A:455:HIS:NE2	5:A:604:HIS:NE2	2.33	0.76
1:B:249:HIS:ND1	7:B:705:HOH:O	2.19	0.76
1:B:263[A]:ASN:CG	7:B:703:HOH:O	2.23	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:TYR:CG	7:B:1088:HOH:O	2.39	0.75
1:A:435:HIS:ND1	5:A:604:HIS:ND1	2.07	0.74
1:A:282:ALA:HA	7:A:1134:HOH:O	1.87	0.73
1:A:263[A]:ASN:OD1	7:A:701:HOH:O	2.07	0.73
1:A:455:HIS:CE1	5:A:604:HIS:NE2	2.58	0.72
1:A:309:LEU:HB2	7:A:1191:HOH:O	1.90	0.71
1:A:309:LEU:HD13	1:A:539:PHE:HB2	1.73	0.71
1:A:455:HIS:NE2	5:A:604:HIS:CG	2.59	0.70
1:A:435:HIS:CE1	5:A:604:HIS:HD1	2.10	0.67
1:B:263[A]:ASN:OD1	7:B:703:HOH:O	2.12	0.66
6:B:602:TRS:O1	7:B:704:HOH:O	2.14	0.65
1:B:354:TYR:CZ	1:B:358[B]:ILE:HD11	2.31	0.65
1:B:294:HIS:HD2	1:B:297:LEU:H	1.44	0.64
1:A:325:ILE:O	6:A:605:TRS:H31	1.98	0.63
1:A:87:ARG:HD2	7:A:1077:HOH:O	1.96	0.63
1:B:407:ILE:O	1:B:411:THR:HB	1.98	0.63
3:A:602:LYS:HG2	7:B:727:HOH:O	1.98	0.62
1:A:282:ALA:C	7:A:717:HOH:O	2.38	0.61
4:A:603:PEG:H41	7:A:1137:HOH:O	2.00	0.61
1:A:309:LEU:HD22	7:A:1191:HOH:O	2.03	0.59
1:B:359[A]:LYS:HE3	7:B:710:HOH:O	2.02	0.59
1:A:455:HIS:CE1	5:A:604:HIS:CD2	2.91	0.58
1:A:460:LYS:HA	7:A:1038:HOH:O	2.03	0.57
1:B:223:MET:O	1:B:225:TYR:O	2.21	0.57
1:A:287:ALA:HA	1:A:332:GLU:OE2	2.05	0.57
1:A:308:GLU:OE1	6:A:606:TRS:O2	2.19	0.57
1:A:435:HIS:HD1	5:A:604:HIS:HD1	0.59	0.55
1:A:435:HIS:HB3	5:A:604:HIS:CE1	2.42	0.54
1:B:249:HIS:CE1	7:B:705:HOH:O	2.57	0.54
1:B:358[A]:ILE:HD13	1:B:492:LEU:HD13	1.90	0.54
1:A:282:ALA:HB3	1:A:302:TYR:CG	2.42	0.54
1:B:359[B]:LYS:NZ	7:B:710:HOH:O	2.32	0.54
1:A:309:LEU:CD1	1:A:539:PHE:HB2	2.39	0.53
1:B:122:LEU:HD21	1:B:128:LEU:HD11	1.90	0.53
1:A:412:ASN:HB2	7:A:760:HOH:O	2.09	0.53
6:A:606:TRS:H22	7:A:906:HOH:O	2.08	0.53
1:A:321[B]:LYS:HE3	3:A:602:LYS:HG3	1.92	0.51
1:A:349:TRP:HE1	3:A:602:LYS:HG3	1.75	0.51
1:A:87:ARG:CD	7:A:1077:HOH:O	2.56	0.51
5:A:604:HIS:O	5:A:604:HIS:CG	2.63	0.51
1:A:275:THR:HB	1:A:276:PRO:HD2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:O	1:A:282:ALA:HB2	2.12	0.50
1:A:279[A]:ASN:ND2	7:A:718:HOH:O	2.45	0.49
1:A:263[A]:ASN:CG	7:A:701:HOH:O	2.47	0.49
1:B:354:TYR:CE2	1:B:358[B]:ILE:HD12	2.48	0.49
1:B:354:TYR:CD2	7:B:1088:HOH:O	2.64	0.49
6:A:606:TRS:C2	7:A:906:HOH:O	2.61	0.49
1:A:183:LYS:CE	7:A:1065:HOH:O	2.60	0.48
1:A:435:HIS:ND1	5:A:604:HIS:CE1	2.72	0.48
1:A:435:HIS:HB3	5:A:604:HIS:HE1	1.77	0.48
1:B:354:TYR:HD2	1:B:355:ASN:OD1	1.97	0.48
1:B:408:GLU:OE1	7:B:706:HOH:O	2.20	0.47
1:B:459:ASN:ND2	7:B:707:HOH:O	2.23	0.47
1:A:412:ASN:ND2	7:A:702:HOH:O	2.21	0.47
1:A:263[B]:ASN:ND2	1:A:267:GLU:OE2	2.46	0.47
1:B:294:HIS:CD2	1:B:297:LEU:H	2.29	0.47
1:A:151:PHE:CE2	1:A:164:LEU:HD21	2.51	0.46
1:A:230:THR:HB	1:A:234:TYR:CE2	2.50	0.46
1:A:349:TRP:HE1	3:A:602:LYS:CG	2.28	0.46
1:A:387:ASN:OD1	1:A:387:ASN:N	2.48	0.46
1:A:455:HIS:NE2	5:A:604:HIS:ND1	2.64	0.46
4:A:603:PEG:H11	1:B:276:PRO:HG2	1.98	0.46
1:B:353:ASP:OD1	1:B:356:ASP:OD2	2.34	0.46
1:B:334:ILE:HG12	1:B:340:PRO:HD3	1.97	0.46
1:A:183:LYS:HE3	7:A:1065:HOH:O	2.16	0.45
1:A:287:ALA:N	7:A:723:HOH:O	2.49	0.45
1:B:354:TYR:CE2	1:B:358[B]:ILE:CD1	3.00	0.45
1:B:225:TYR:O	1:B:227:LEU:N	2.50	0.45
1:A:150:ARG:HB2	1:A:165:ALA:HB3	1.99	0.45
1:B:147:GLN:C	1:B:149:LEU:H	2.20	0.44
1:B:502:LEU:HD23	1:B:502:LEU:C	2.38	0.44
1:B:518:PHE:CD2	1:B:518:PHE:C	2.91	0.43
5:A:604:HIS:ND1	5:A:604:HIS:O	2.51	0.43
1:B:351:TYR:O	6:B:602:TRS:H11	2.18	0.43
1:A:282:ALA:HB3	1:A:302:TYR:CB	2.49	0.43
1:B:143:SER:HB2	1:B:151:PHE:HB2	2.00	0.43
1:B:518:PHE:C	1:B:518:PHE:HD2	2.22	0.43
1:B:87:ARG:HD2	7:B:1053:HOH:O	2.18	0.43
1:B:227:LEU:HD11	1:B:232:ILE:HG21	2.02	0.42
4:A:603:PEG:O1	7:A:703:HOH:O	2.21	0.42
1:B:124:ASN:O	1:B:126:GLU:N	2.52	0.42
7:A:973:HOH:O	1:B:294:HIS:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279[B]:ASN:HD21	1:A:282:ALA:HB2	1.85	0.42
1:B:222:PRO:HD2	1:B:243:ILE:HD11	2.02	0.41
1:B:437:ILE:HD11	1:B:455:HIS:CG	2.54	0.41
1:B:502:LEU:HA	1:B:554:GLY:O	2.21	0.41
1:B:417:GLN:HA	1:B:418:PRO:C	2.40	0.41
1:A:275:THR:HB	1:A:276:PRO:CD	2.50	0.41
1:A:277[A]:MET:HE3	1:A:304:ARG:NH2	2.36	0.41
1:A:502:LEU:HD12	1:A:555:LEU:CD2	2.51	0.41
1:B:108:ARG:NH2	7:B:727:HOH:O	2.44	0.41
1:B:353:ASP:HB3	7:B:831:HOH:O	1.90	0.40
1:B:457:ILE:HD13	1:B:457:ILE:HG21	1.89	0.40
1:B:477:PRO:HD2	7:B:944:HOH:O	2.21	0.40
1:A:382:LYS:NZ	7:A:735:HOH:O	2.52	0.40
1:A:83:TYR:CG	1:A:220:MET:HG3	2.57	0.40
1:B:442:PRO:HA	1:B:443:PRO:HD3	1.91	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)
7:A:1167:HOH:O	7:B:1149:HOH:O[3_544]	2.09	0.11

## 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	493/507 (97%)	483 (98%)	9 (2%)	1 (0%)	47 26
1	B	488/507 (96%)	471 (96%)	13 (3%)	4 (1%)	19 5
All	All	981/1014 (97%)	954 (97%)	22 (2%)	5 (0%)	29 11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	B	224	LYS
1	B	125	GLY
1	B	148	LYS
1	B	226	GLY

### 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	451/457 (99%)	444 (98%)	7 (2%)	62	40
1	B	432/457 (94%)	422 (98%)	10 (2%)	50	24
All	All	883/914 (97%)	866 (98%)	17 (2%)	55	32

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASP
1	A	142	VAL
1	A	160	LYS
1	A	280	LEU
1	A	387	ASN
1	A	492	LEU
1	A	579	MET
1	B	78	VAL
1	B	108	ARG
1	B	147	GLN
1	B	149	LEU
1	B	174	LYS
1	B	411	THR
1	B	438	GLU
1	B	450	ASP
1	B	492	LEU
1	B	518	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	568	ASN
1	B	127	HIS
1	B	294	HIS
1	B	387	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	TRS	B	602	-	7,7,7	0.79	0	9,9,9	1.49	2 (22%)
6	TRS	B	603	-	7,7,7	1.66	2 (28%)	9,9,9	1.95	4 (44%)
4	PEG	A	603	-	6,6,6	0.53	0	5,5,5	0.79	0
6	TRS	A	605	-	7,7,7	1.59	3 (42%)	9,9,9	2.23	4 (44%)
2	FYB	A	601	-	23,27,27	2.72	7 (30%)	25,41,41	3.74	12 (48%)
6	TRS	A	606	-	7,7,7	1.00	0	9,9,9	1.04	0
2	FYB	B	601	-	23,27,27	1.77	7 (30%)	25,41,41	4.29	12 (48%)

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
6	TRS	B	602	-	-	3/9/9/9	-
6	TRS	B	603	-	-	6/9/9/9	-
4	PEG	A	603	-	-	3/4/4/4	-
6	TRS	A	605	-	-	6/9/9/9	-
2	FYB	A	601	-	-	0/8/24/24	0/3/3/3
6	TRS	A	606	-	-	4/9/9/9	-
2	FYB	B	601	-	-	0/8/24/24	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FYB	C4-C3	6.94	1.57	1.50
2	A	601	FYB	C1-C	5.41	1.58	1.52
2	A	601	FYB	C8-C7	4.82	1.57	1.49
2	A	601	FYB	C2-C3	4.75	1.55	1.50
2	B	601	FYB	F1-C3	-3.73	1.31	1.38
2	A	601	FYB	C1-C2	3.64	1.64	1.53
2	A	601	FYB	C11-C16	-3.42	1.36	1.41
2	B	601	FYB	C4-C3	2.98	1.53	1.50
6	B	603	TRS	O1-C1	2.87	1.51	1.42
2	B	601	FYB	C9-C10	2.86	1.43	1.37
2	B	601	FYB	C8-C7	2.72	1.53	1.49
6	A	605	TRS	O3-C3	-2.68	1.33	1.42
2	B	601	FYB	C1-C2	2.52	1.60	1.53
2	B	601	FYB	C14-C13	2.43	1.41	1.37
2	A	601	FYB	C7-N	-2.36	1.28	1.33
6	A	605	TRS	O1-C1	2.13	1.49	1.42
6	B	603	TRS	O3-C3	2.10	1.49	1.42
2	B	601	FYB	C2-C3	2.05	1.52	1.50
6	A	605	TRS	C3-C	-2.02	1.46	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FYB	C1-C2-C3	-13.76	102.77	110.93
2	A	601	FYB	C1-C2-C3	-10.09	104.94	110.93
2	B	601	FYB	F-C3-C4	-9.84	102.96	109.37
2	A	601	FYB	C5-C4-C3	9.48	116.56	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FYB	C9-C10-C11	-6.96	115.34	123.05
2	A	601	FYB	F1-C3-C2	6.87	113.84	109.37
2	B	601	FYB	F1-C3-C2	5.64	113.04	109.37
2	A	601	FYB	F-C3-C2	-5.14	106.02	109.37
2	A	601	FYB	C9-C10-C11	-4.68	117.86	123.05
2	B	601	FYB	O3-C8-C9	4.40	124.64	119.15
6	B	603	TRS	C2-C-C1	3.65	122.13	110.81
2	B	601	FYB	F-C3-C2	-3.63	107.00	109.37
6	B	602	TRS	C2-C-N	3.48	118.37	107.98
6	A	605	TRS	C3-C-C2	-3.28	100.63	110.81
2	B	601	FYB	C5-C-C1	3.21	113.61	109.85
2	A	601	FYB	C2-C1-C	3.16	117.45	111.25
2	A	601	FYB	O3-C8-C9	3.11	123.02	119.15
6	A	605	TRS	C2-C-N	3.07	117.14	107.98
2	B	601	FYB	O3-C16-C11	-2.87	118.43	121.20
2	B	601	FYB	F2-C13-C12	-2.78	114.99	119.17
2	A	601	FYB	O-C-C5	-2.75	101.64	108.19
6	A	605	TRS	C3-C-C1	2.71	119.20	110.81
6	A	605	TRS	C3-C-N	-2.69	99.94	107.98
2	B	601	FYB	F1-C3-C4	2.55	111.03	109.37
6	B	603	TRS	C3-C-C1	-2.54	102.94	110.81
2	A	601	FYB	O1-C7-N	2.51	127.61	122.61
2	A	601	FYB	C13-C12-C11	2.48	121.20	119.43
6	B	603	TRS	O2-C2-C	2.31	118.31	111.00
2	B	601	FYB	O1-C7-N	2.24	127.07	122.61
2	A	601	FYB	C14-C13-C12	-2.23	120.77	123.23
2	A	601	FYB	F2-C13-C14	2.17	122.23	118.54
6	B	603	TRS	C3-C-C2	-2.09	104.34	110.81
6	B	602	TRS	C3-C-C2	-2.05	104.46	110.81
2	B	601	FYB	F2-C13-C14	2.04	122.00	118.54

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	602	TRS	C1-C-C2-O2
6	B	602	TRS	C3-C-C2-O2
6	B	603	TRS	C2-C-C1-O1
6	B	603	TRS	C3-C-C1-O1
6	B	603	TRS	N-C-C1-O1
6	B	603	TRS	C3-C-C2-O2
6	B	603	TRS	N-C-C2-O2

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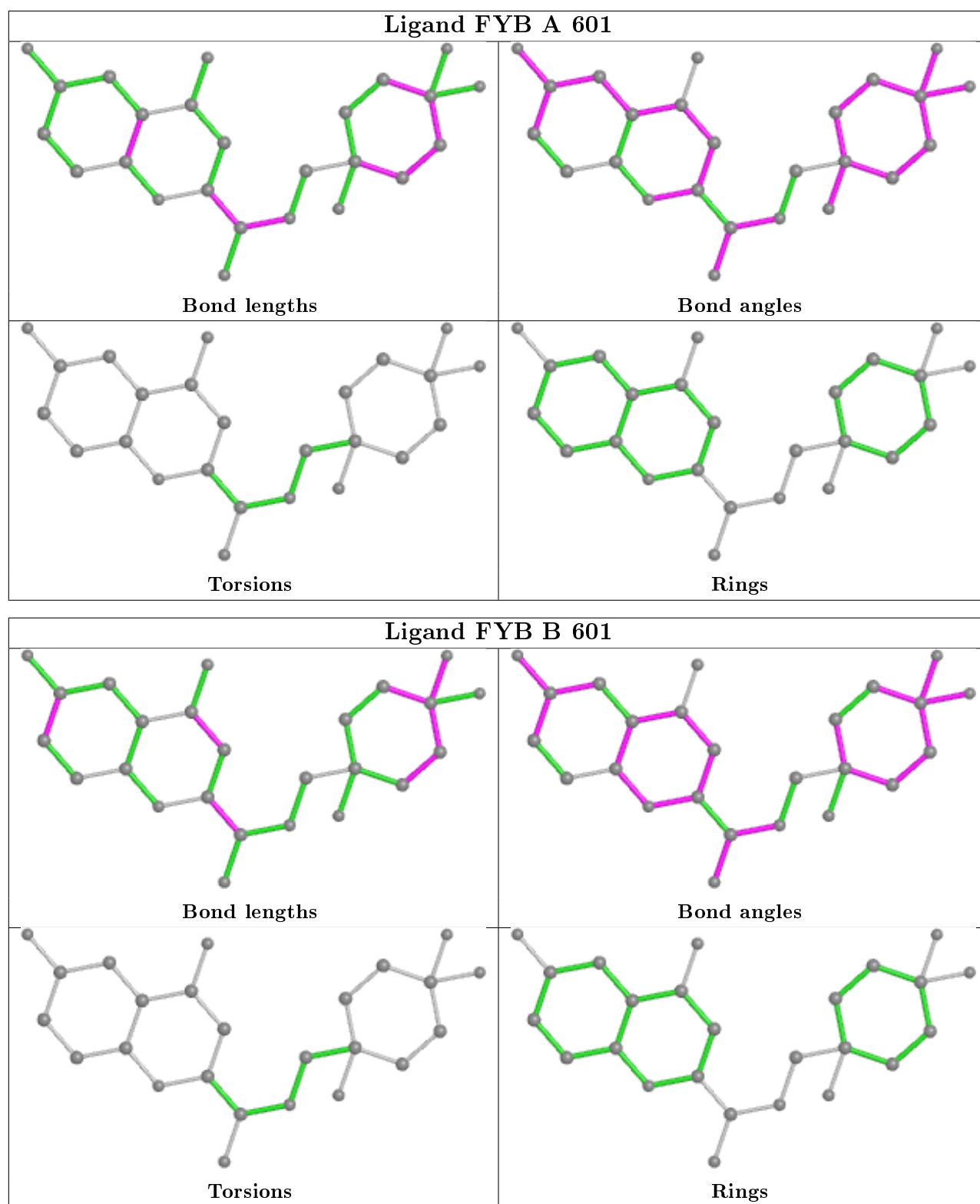
Mol	Chain	Res	Type	Atoms
6	A	605	TRS	N-C-C2-O2
6	A	605	TRS	C1-C-C3-O3
6	A	605	TRS	C2-C-C3-O3
6	A	605	TRS	N-C-C3-O3
4	A	603	PEG	O1-C1-C2-O2
4	A	603	PEG	O2-C3-C4-O4
6	B	602	TRS	N-C-C2-O2
6	B	603	TRS	C1-C-C2-O2
6	A	605	TRS	C3-C-C1-O1
6	A	606	TRS	N-C-C2-O2
6	A	606	TRS	C2-C-C3-O3
4	A	603	PEG	C1-C2-O2-C3
6	A	605	TRS	C2-C-C1-O1
6	A	606	TRS	C1-C-C2-O2
6	A	606	TRS	C3-C-C2-O2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	602	TRS	3	0
4	A	603	PEG	3	0
6	A	605	TRS	1	0
6	A	606	TRS	3	0

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



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	485/507 (95%)	-0.31	9 (1%) 66 65	10, 21, 45, 74	0
1	B	485/507 (95%)	-0.13	7 (1%) 75 74	9, 24, 56, 77	0
All	All	970/1014 (95%)	-0.22	16 (1%) 72 71	9, 22, 53, 77	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	5.6
1	A	145	SER	5.6
1	A	78	VAL	5.0
1	A	535	LEU	4.5
1	A	225	TYR	3.9
1	A	518	PHE	3.6
1	B	78	VAL	3.3
1	B	147	GLN	2.9
1	B	354	TYR	2.9
1	B	227	LEU	2.8
1	A	536	ASP	2.6
1	A	144	ALA	2.2
1	A	517[A]	CYS	2.1
1	A	354	TYR	2.1
1	B	169	PHE	2.0
1	B	230	THR	2.0

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

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

### 6.3 Carbohydrates

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.

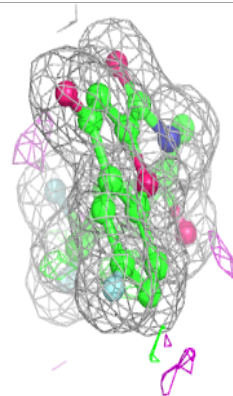
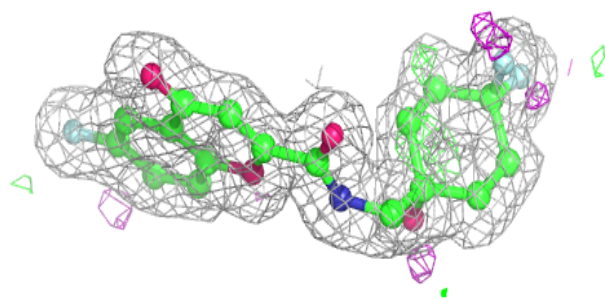
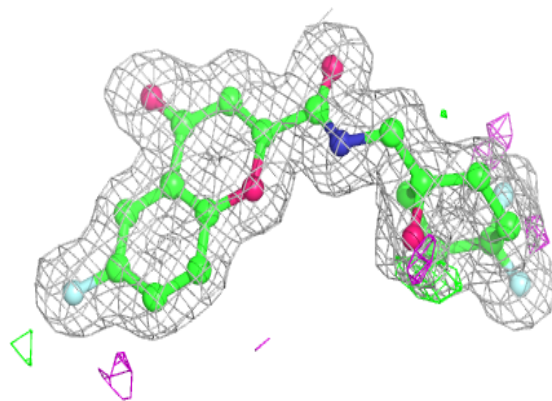
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	LYS	A	602	8/10	0.70	0.21	39,46,52,58	0
6	TRS	B	602	8/8	0.81	0.22	40,47,50,64	0
4	PEG	A	603	7/7	0.84	0.12	41,46,52,54	0
6	TRS	A	606	8/8	0.84	0.20	25,28,31,47	0
6	TRS	B	603	8/8	0.87	0.10	22,28,35,40	0
5	HIS	A	604	10/11	0.92	0.22	13,41,58,62	0
6	TRS	A	605	8/8	0.93	0.15	21,28,32,41	1
2	FYB	A	601	25/25	0.96	0.07	13,16,20,22	0
2	FYB	B	601	25/25	0.96	0.07	14,17,20,23	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.

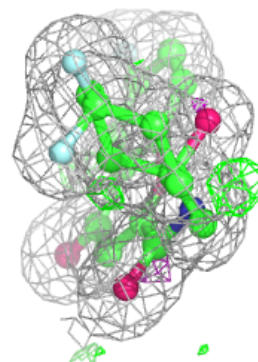
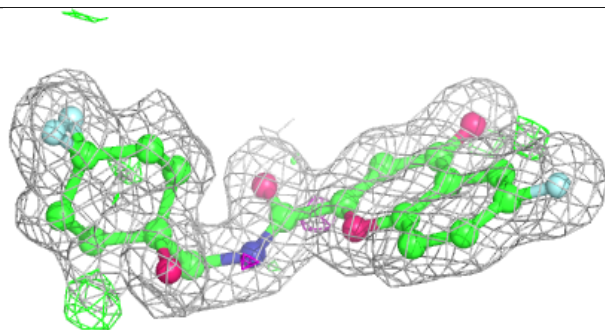
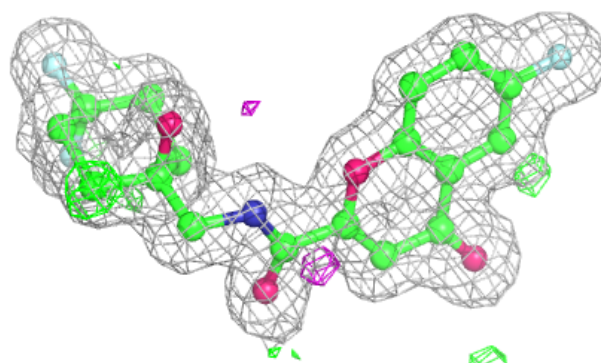


**Electron density around FYB A 601:**

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

**Electron density around FYB 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.