



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:01 AM UTC

PDB ID : 6HCU / pdb_00006hcu
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

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

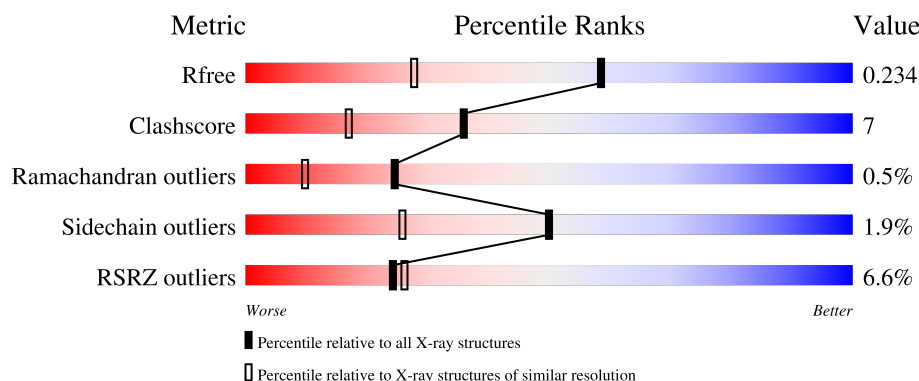
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (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 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	507	5% 80% 13% • •
1	B	507	8% 79% 14% • •

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](#)

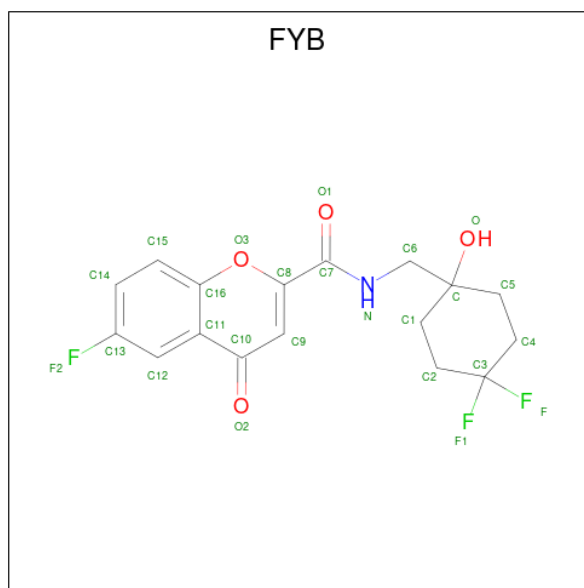
There are 7 unique types of molecules in this entry. The entry contains 9037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

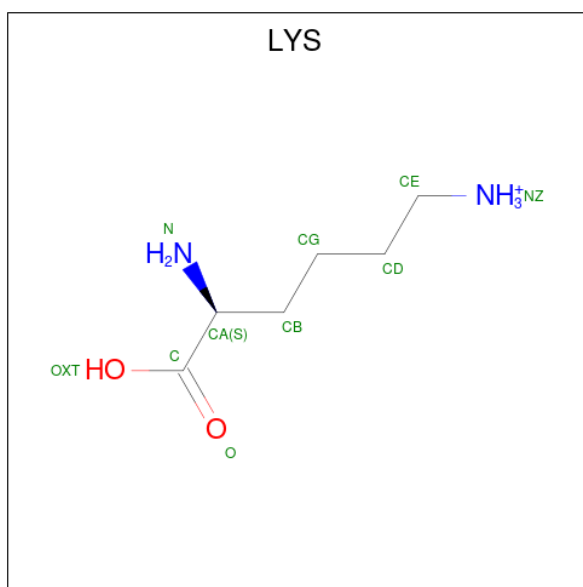
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	13	0
			4015	2598	663	731	23			
1	B	485	Total	C	N	O	S	0	9	0
			3949	2558	652	719	20			

- Molecule 2 is {N}-[[4,4-bis(fluoranyl)-1-oxidanyl-cyclohexyl]methyl]-6-fluoranyl-4-oxidanylidene-chromene-2-carboxamide (CCD ID: FYB) (formula: C₁₇H₁₆F₃NO₄).



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 (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



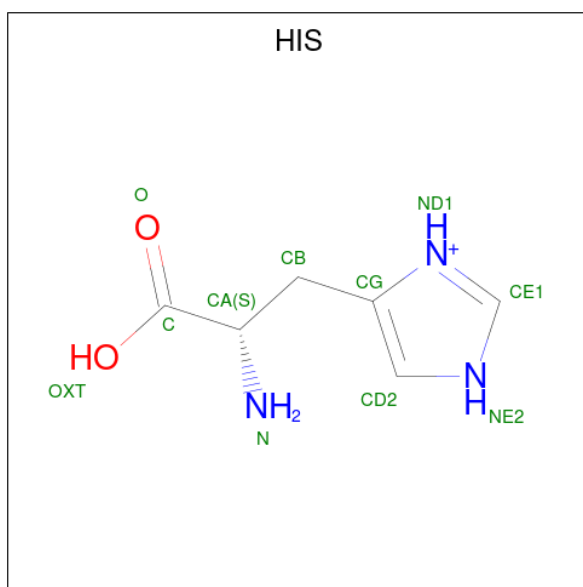
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



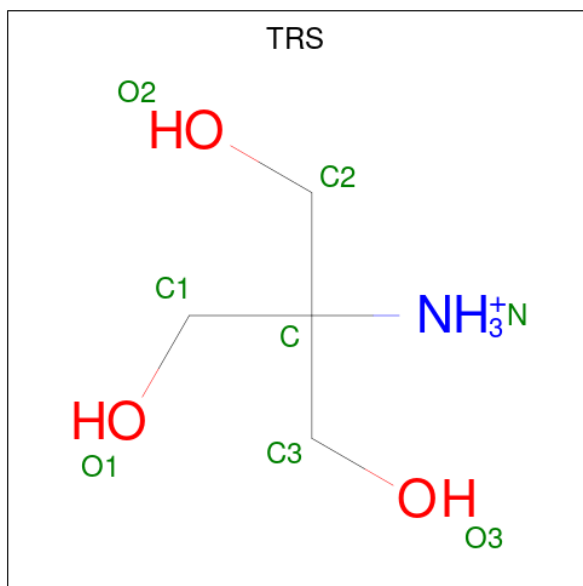
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is HISTIDINE (CCD ID: HIS) (formula: $C_6H_{10}N_3O_2$).



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 (CCD ID: 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		

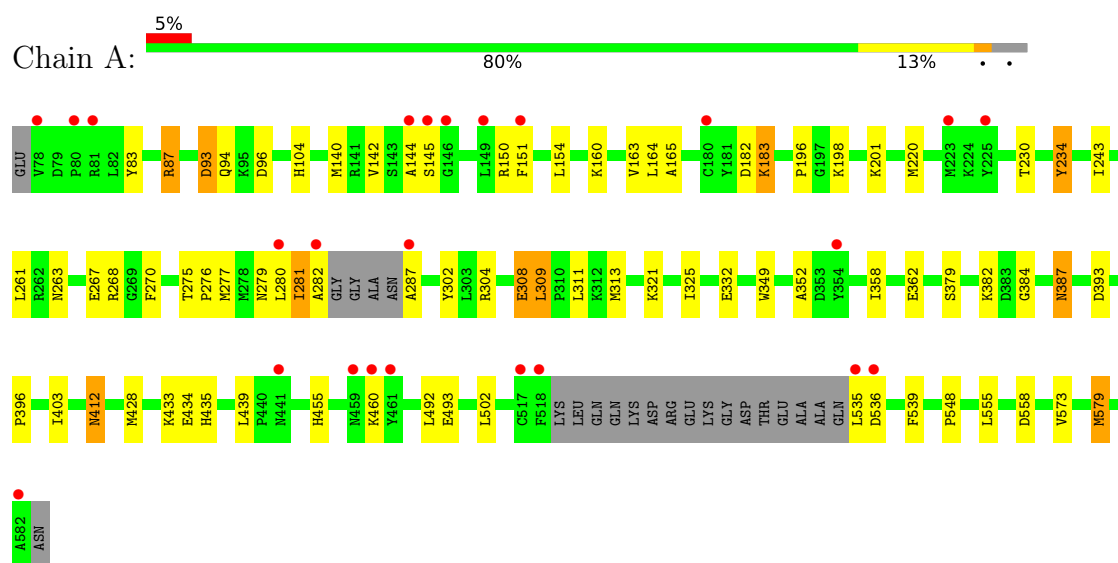
- Molecule 7 is water.

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

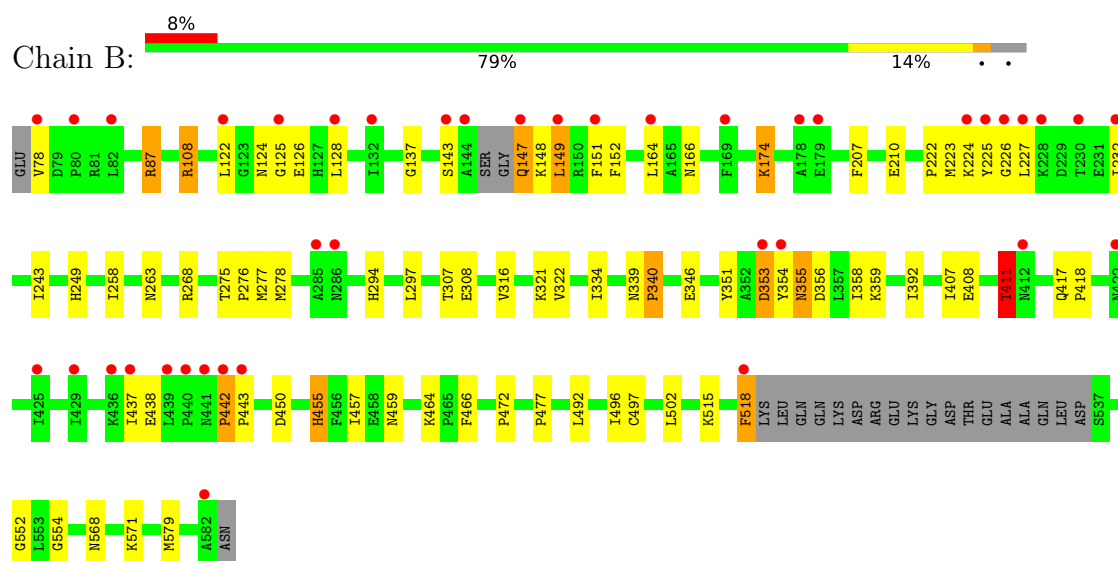
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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, α , β , γ	73.14Å 95.34Å 166.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.74 – 1.62 82.74 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.3 (82.74-1.62) 99.3 (82.74-1.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.183 , 0.226 0.194 , 0.234	Depositor DCC
R_{free} test set	7338 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: PEG, FYB, TRS

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	1.52	26/4155 (0.6%)	1.32	21/5612 (0.4%)
1	B	1.46	24/4073 (0.6%)	1.30	13/5508 (0.2%)
All	All	1.49	50/8228 (0.6%)	1.31	34/11120 (0.3%)

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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	GLU	N-CA	-7.07	1.37	1.46
1	A	393	ASP	N-CA	-7.00	1.37	1.46
1	A	439	LEU	CA-C	-6.94	1.45	1.52
1	B	568	ASN	CA-CB	6.92	1.65	1.53
1	B	278	MET	N-CA	6.92	1.54	1.46
1	A	196	PRO	CA-C	6.53	1.59	1.52
1	B	164	LEU	N-CA	6.44	1.54	1.46
1	A	548	PRO	C-O	-6.09	1.17	1.24
1	B	275	THR	C-O	-6.09	1.19	1.24
1	A	261	LEU	CA-C	-6.05	1.45	1.52
1	B	322	VAL	C-O	-5.88	1.18	1.24
1	B	166	ASN	N-CA	5.86	1.53	1.46
1	A	270	PHE	N-CA	5.83	1.53	1.45
1	B	87	ARG	CD-NE	-5.83	1.38	1.46
1	A	87	ARG	CD-NE	-5.70	1.38	1.46
1	A	154	LEU	CA-CB	-5.65	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	TYR	CA-C	-5.64	1.44	1.52
1	B	316	VAL	C-O	5.63	1.30	1.24
1	B	392	ILE	C-O	-5.60	1.18	1.24
1	B	552	GLY	N-CA	5.57	1.51	1.45
1	B	355	ASN	N-CA	-5.53	1.39	1.46
1	A	396	PRO	CA-C	5.52	1.57	1.52
1	B	307	THR	C-O	5.47	1.31	1.24
1	A	428	MET	CA-C	5.46	1.59	1.52
1	A	412	ASN	CG-OD1	5.44	1.33	1.23
1	B	571	LYS	CA-C	-5.39	1.45	1.52
1	A	104	HIS	C-O	5.37	1.30	1.24
1	A	140	MET	C-O	-5.35	1.17	1.24
1	B	515	LYS	N-CA	5.34	1.52	1.46
1	B	579	MET	N-CA	5.31	1.52	1.45
1	A	379	SER	N-CA	-5.29	1.39	1.46
1	B	466	PHE	N-CA	5.28	1.52	1.45
1	B	207	PHE	N-CA	5.26	1.52	1.46
1	A	243	ILE	N-CA	5.26	1.52	1.46
1	A	433	LYS	N-CA	5.26	1.52	1.46
1	B	496	ILE	N-CA	5.24	1.53	1.46
1	A	96	ASP	N-CA	5.22	1.52	1.46
1	B	450	ASP	C-O	-5.22	1.18	1.24
1	B	152	PHE	N-CA	5.21	1.52	1.45
1	A	182	ASP	CA-C	5.18	1.59	1.52
1	A	311	LEU	N-CA	5.17	1.52	1.46
1	B	472	PRO	C-O	5.17	1.29	1.23
1	A	198	LYS	N-CA	-5.12	1.39	1.45
1	B	268	ARG	CZ-NH1	5.08	1.39	1.32
1	B	137	GLY	N-CA	5.06	1.50	1.45
1	B	353	ASP	CB-CG	5.06	1.64	1.52
1	A	558	ASP	N-CA	5.04	1.52	1.46
1	A	573	VAL	N-CA	5.03	1.51	1.46
1	A	362	GLU	C-O	5.03	1.30	1.24
1	A	94	GLN	N-CA	-5.00	1.40	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	HIS	N-CA-C	9.61	121.36	111.07
1	A	281	ILE	N-CA-C	-9.27	94.80	108.89
1	A	384	GLY	CA-C-N	7.61	127.33	119.56
1	A	384	GLY	C-N-CA	7.61	127.33	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ASP	N-CA-C	6.83	119.31	111.11
1	B	455	HIS	N-CA-C	6.45	118.11	111.14
1	B	87	ARG	NE-CZ-NH2	-6.41	113.43	119.20
1	A	439	LEU	CA-C-N	-6.40	114.04	120.31
1	A	439	LEU	C-N-CA	-6.40	114.04	120.31
1	A	434	GLU	N-CA-C	6.35	119.01	111.71
1	B	411	THR	N-CA-CB	-6.24	101.25	110.49
1	A	352	ALA	O-C-N	6.15	129.95	123.06
1	A	87	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	A	183	LYS	CB-CA-C	-5.80	97.87	109.99
1	A	87	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	B	346	GLU	CB-CG-CD	5.75	122.37	112.60
1	B	353	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	464	LYS	CA-C-N	-5.74	114.35	120.03
1	B	464	LYS	C-N-CA	-5.74	114.35	120.03
1	A	493	GLU	N-CA-CB	-5.59	101.42	110.81
1	A	403	ILE	N-CA-C	5.49	115.69	110.42
1	A	268	ARG	N-CA-C	5.40	119.50	113.02
1	B	308	GLU	N-CA-C	5.32	117.49	111.11
1	B	497	CYS	N-CA-C	5.30	118.51	111.30
1	B	442	PRO	CA-C-N	5.29	126.45	119.84
1	B	442	PRO	C-N-CA	5.29	126.45	119.84
1	A	579	MET	CA-CB-CG	5.20	124.50	114.10
1	B	258	ILE	N-CA-C	5.08	115.80	110.62
1	A	183	LYS	CB-CG-CD	-5.08	99.62	111.30
1	B	339	ASN	CB-CA-C	5.08	116.27	109.42
1	A	163	VAL	O-C-N	5.05	129.00	123.10
1	A	358	ILE	CB-CA-C	-5.01	105.56	111.97
1	A	309	LEU	CA-C-N	-5.01	113.88	119.19
1	A	309	LEU	C-N-CA	-5.01	113.88	119.19

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

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	60	0
1	B	3949	0	3908	50	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	22	1
7	B	451	0	0	21	1
All	All	9037	0	7996	117	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 (117) 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:CG	7:B:703:HOH:O	2.23	0.80
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD11	1:A:313[B]:MET:HE3	1.73	0.69
1:A:435:HIS:CE1	5:A:604:HIS:HD1	2.10	0.67
1:A:282:ALA:C	7:A:717:HOH:O	2.38	0.66
6:B:602:TRS:O1	7:B:704:HOH:O	2.14	0.65
1:B:263[A]:ASN:OD1	7:B:703:HOH:O	2.12	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
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:277[B]:MET:HE3	1:B:277[B]:MET:HE2	1.86	0.56
1:B:359[B]:LYS:NZ	7:B:710:HOH:O	2.32	0.56
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:A:263[A]:ASN:CG	7:A:701:HOH:O	2.47	0.54
1:A:277[B]:MET:HE3	1:B:277[B]:MET:CE	2.38	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: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:CG	5:A:604:HIS:O	2.63	0.51
1:A:275:THR:HB	1:A:276:PRO:HD2	1.91	0.50
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:B:354:TYR:CE2	1:B:358[B]:ILE:HD12	2.48	0.49
1:B:147:GLN:C	1:B:149:LEU:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:518:PHE:C	1:B:518:PHE:CD2	2.91	0.49
1:B:502:LEU:C	1:B:502:LEU:HD23	2.38	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:518:PHE:C	1:B:518:PHE:HD2	2.22	0.47
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:B:417:GLN:HA	1:B:418:PRO:C	2.40	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:A:277[A]:MET:HE3	1:A:304:ARG:CZ	2.48	0.44
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: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:A:201:LYS:NZ	7:A:728:HOH:O	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ILE:HD11	1:B:455:HIS:CG	2.54	0.41
1:A:535:LEU:O	1:A:536:ASP:C	2.63	0.41
1:A:277[A]:MET:HE3	1:A:304:ARG:NH2	2.36	0.41
1:B:502:LEU:HA	1:B:554:GLY:O	2.21	0.41
1:A:275:THR:HB	1:A:276:PRO:CD	2.50	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:174:LYS:HD3	1:B:210:GLU:CD	2.46	0.40
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:309:LEU:HG	1:A:313[A]:MET:HE2	2.03	0.40
1:A:83:TYR:CG	1:A:220:MET:HG3	2.57	0.40
1:A:382:LYS:NZ	7:A:735:HOH:O	2.52	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%)	43	25
1	B	488/507 (96%)	471 (96%)	13 (3%)	4 (1%)	16	4
All	All	981/1014 (97%)	954 (97%)	22 (2%)	5 (0%)	24	10

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%)	55	32
1	B	432/457 (94%)	423 (98%)	9 (2%)	47	22
All	All	883/914 (97%)	867 (98%)	16 (2%)	50	28

All (16) 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	340	PRO
1	B	411	THR
1	B	438	GLU
1	B	518	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	127	HIS
1	B	134	ASN
1	B	162	GLN
1	B	294	HIS
1	B	387	ASN
1	B	451	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 ⓘ

There are no oligosaccharides 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	A	606	-	7,7,7	1.05	0	9,9,9	1.19	1 (11%)
6	TRS	B	603	-	7,7,7	1.76	2 (28%)	9,9,9	2.26	4 (44%)
2	FYB	A	601	-	27,27,27	2.14	8 (29%)	34,41,41	1.42	6 (17%)
3	LYS	A	602	-	6,7,9	1.09	1 (16%)	5,8,10	1.16	0
6	TRS	A	605	-	7,7,7	1.70	3 (42%)	9,9,9	2.60	5 (55%)
6	TRS	B	602	-	7,7,7	0.86	0	9,9,9	1.73	2 (22%)
4	PEG	A	603	-	6,6,6	0.54	0	5,5,5	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FYB	B	601	-	27,27,27	1.37	4 (14%)	34,41,41	2.04	14 (41%)
5	HIS	A	604	-	9,10,11	1.01	0	8,12,14	0.97	0

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	A	606	-	-	5/9/9/9	-
6	TRS	B	603	-	-	6/9/9/9	-
2	FYB	A	601	-	-	0/10/24/24	0/3/3/3
3	LYS	A	602	-	-	5/7/7/9	-
6	TRS	A	605	-	-	7/9/9/9	-
6	TRS	B	602	-	-	3/9/9/9	-
4	PEG	A	603	-	-	3/4/4/4	-
2	FYB	B	601	-	-	0/10/24/24	0/3/3/3
5	HIS	A	604	-	-	1/5/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FYB	C1-C	5.42	1.58	1.52
2	A	601	FYB	C8-C7	4.89	1.57	1.47
2	A	601	FYB	C1-C2	3.82	1.64	1.53
2	A	601	FYB	C4-C3	3.32	1.57	1.50
2	B	601	FYB	C8-C7	3.27	1.53	1.47
2	A	601	FYB	C7-N	-2.99	1.28	1.33
6	B	603	TRS	O1-C1	2.98	1.51	1.42
6	A	605	TRS	O3-C3	-2.80	1.33	1.42
2	B	601	FYB	C1-C2	2.64	1.60	1.53
3	A	602	LYS	OXT-C	-2.48	1.22	1.30
2	A	601	FYB	C9-C10	-2.44	1.39	1.44
2	B	601	FYB	C14-C13	2.40	1.41	1.37
6	A	605	TRS	C3-C	-2.32	1.46	1.53
2	A	601	FYB	C11-C16	-2.23	1.36	1.40
6	A	605	TRS	O1-C1	2.22	1.49	1.42
2	A	601	FYB	C2-C3	2.21	1.55	1.50
6	B	603	TRS	O3-C3	2.18	1.49	1.42
2	B	601	FYB	O3-C8	-2.14	1.33	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FYB	C4-C3-C2	4.91	119.21	114.33
6	B	603	TRS	C2-C-C1	4.31	122.13	110.66
6	B	602	TRS	C2-C-N	4.00	118.37	108.17
6	A	605	TRS	C3-C-C2	-3.77	100.63	110.66
2	B	601	FYB	O2-C10-C11	3.63	126.51	121.38
6	A	605	TRS	C2-C-N	3.52	117.14	108.17
2	B	601	FYB	F-C3-C4	-3.45	102.96	108.92
2	B	601	FYB	O3-C16-C11	-3.45	118.43	121.57
2	B	601	FYB	C5-C-C1	3.37	113.61	109.68
6	A	605	TRS	C3-C-N	-3.23	99.94	108.17
6	A	605	TRS	C3-C-C1	3.21	119.20	110.66
2	A	601	FYB	C2-C1-C	3.20	117.45	111.25
6	B	603	TRS	C3-C-C1	-2.90	102.94	110.66
2	A	601	FYB	F1-C3-C2	2.86	113.84	108.92
2	A	601	FYB	O-C-C5	-2.76	101.64	108.25
6	B	603	TRS	O2-C2-C	2.67	118.31	110.88
2	B	601	FYB	O1-C7-C8	-2.62	116.99	121.10
2	B	601	FYB	O2-C10-C9	-2.44	117.97	121.88
2	B	601	FYB	F1-C3-C2	2.39	113.04	108.92
2	B	601	FYB	C16-C11-C10	2.39	121.29	119.74
6	B	603	TRS	C3-C-C2	-2.37	104.34	110.66
2	A	601	FYB	O1-C7-N	2.36	127.61	123.35
6	B	602	TRS	C3-C-C2	-2.33	104.46	110.66
2	B	601	FYB	F2-C13-C12	-2.31	114.99	118.28
2	A	601	FYB	F2-C13-C14	2.30	122.23	118.55
2	B	601	FYB	C15-C16-C11	2.30	124.21	119.94
2	B	601	FYB	F2-C13-C14	2.15	122.00	118.55
6	A	605	TRS	O1-C1-C	2.10	116.74	110.88
6	A	606	TRS	O3-C3-C	-2.07	105.09	110.88
2	B	601	FYB	O1-C7-N	2.06	127.07	123.35
2	B	601	FYB	C6-N-C7	-2.04	120.13	122.73
2	A	601	FYB	C11-C12-C13	2.03	121.20	117.93

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	LYS	C-CA-CB-CG
3	A	602	LYS	CA-CB-CG-CD
5	A	604	HIS	C-CA-CB-CG
6	A	605	TRS	N-C-C2-O2

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

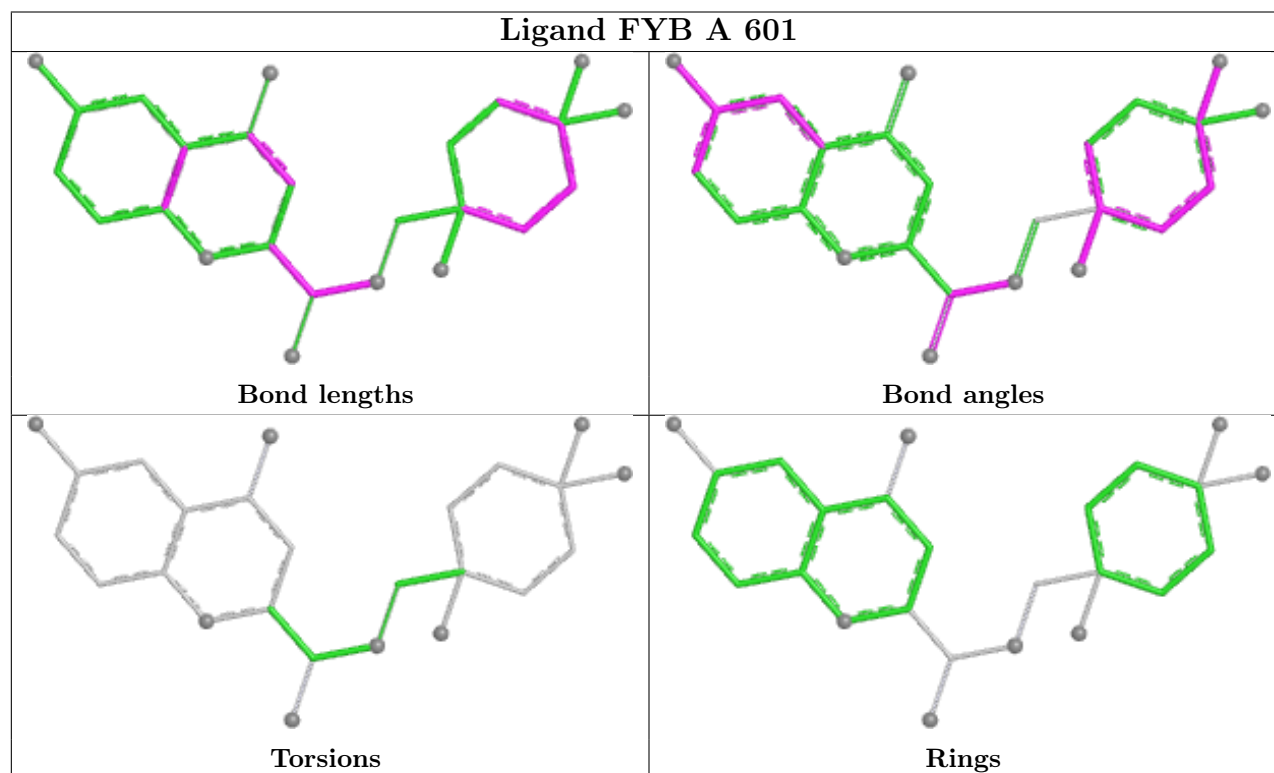
There are no ring outliers.

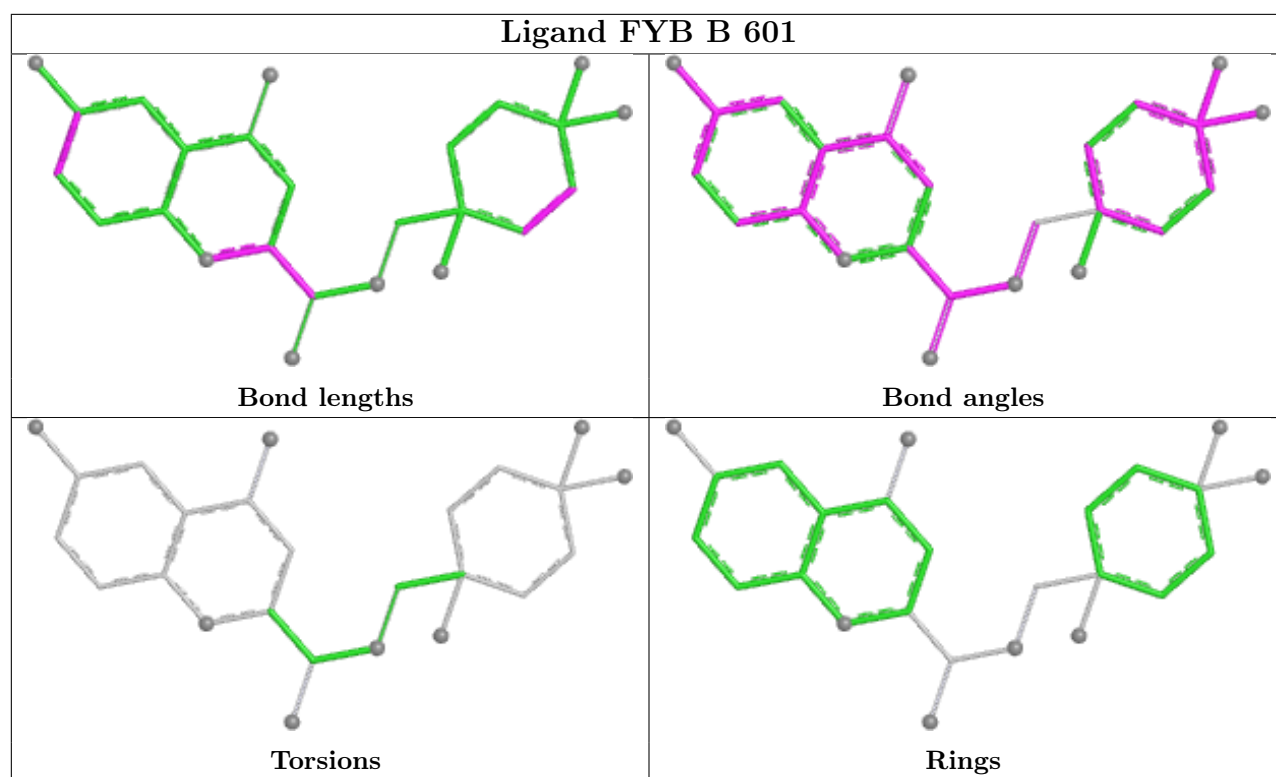
6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	TRS	3	0
3	A	602	LYS	5	0
6	A	605	TRS	1	0
6	B	602	TRS	3	0
4	A	603	PEG	3	0
5	A	604	HIS	16	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 [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, 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	485/507 (95%)	0.09	24 (4%)	35 37	8, 21, 45, 74	13 (2%)
1	B	485/507 (95%)	0.35	40 (8%)	17 18	7, 24, 56, 77	9 (1%)
All	All	970/1014 (95%)	0.22	64 (6%)	24 26	7, 22, 53, 77	22 (2%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	6.6
1	B	78	VAL	6.1
1	A	518	PHE	5.2
1	A	535	LEU	5.1
1	A	78	VAL	4.8
1	B	582	ALA	4.8
1	B	354	TYR	4.6
1	B	518	PHE	4.3
1	B	227	LEU	4.2
1	A	145	SER	3.9
1	A	225	TYR	3.9
1	B	225	TYR	3.8
1	B	440	PRO	3.7
1	B	230	THR	3.5
1	B	437	ILE	3.5
1	B	149	LEU	3.5
1	A	354	TYR	3.5
1	B	439	LEU	3.3
1	A	582	ALA	3.2
1	A	280	LEU	3.1
1	B	147	GLN	3.1
1	A	517[A]	CYS	3.0
1	B	80	PRO	3.0
1	A	151	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	169	PHE	2.9
1	A	144	ALA	2.9
1	B	82	LEU	2.9
1	B	151	PHE	2.8
1	B	442	PRO	2.8
1	B	122	LEU	2.8
1	B	164	LEU	2.7
1	B	226	GLY	2.7
1	B	285	ALA	2.7
1	A	461	TYR	2.7
1	B	128	LEU	2.7
1	B	443	PRO	2.6
1	A	149	LEU	2.6
1	B	228	LYS	2.6
1	A	223	MET	2.6
1	B	179	GLU	2.6
1	B	132	ILE	2.5
1	A	536	ASP	2.5
1	B	224	LYS	2.5
1	B	353	ASP	2.4
1	B	286	ASN	2.4
1	A	460	LYS	2.3
1	B	143	SER	2.3
1	B	125	GLY	2.3
1	B	422	ASN	2.3
1	B	441	ASN	2.3
1	B	178	ALA	2.2
1	A	80	PRO	2.2
1	A	441	ASN	2.2
1	A	146	GLY	2.1
1	A	459	ASN	2.1
1	A	81	ARG	2.1
1	B	429	ILE	2.1
1	A	282	ALA	2.1
1	B	425	ILE	2.1
1	A	287	ALA	2.0
1	B	412	ASN	2.0
1	B	232	ILE	2.0
1	A	180[A]	CYS	2.0
1	B	436	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 [i](#)

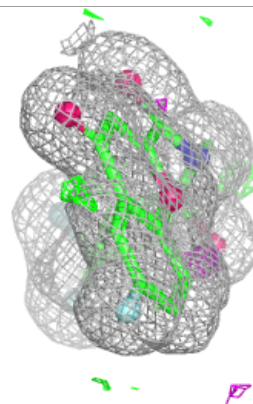
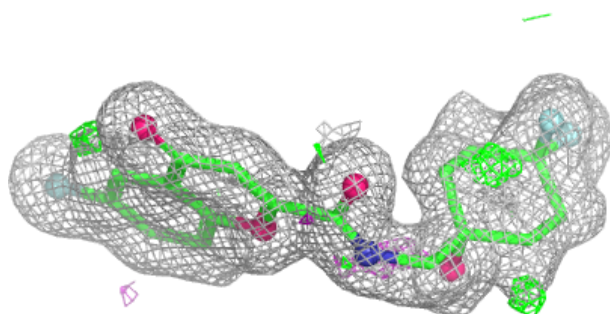
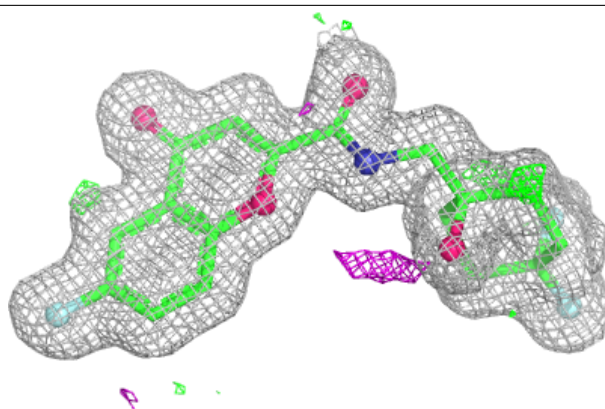
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LYS	A	602	8/10	0.78	0.17	39,46,52,58	0
6	TRS	B	602	8/8	0.81	0.15	40,47,50,64	0
4	PEG	A	603	7/7	0.82	0.17	41,46,52,54	0
6	TRS	A	606	8/8	0.86	0.14	25,28,31,47	0
6	TRS	B	603	8/8	0.87	0.13	22,28,35,40	0
5	HIS	A	604	10/11	0.90	0.18	13,41,58,62	0
6	TRS	A	605	8/8	0.91	0.12	21,28,32,41	1
2	FYB	B	601	25/25	0.96	0.06	14,17,20,23	0
2	FYB	A	601	25/25	0.96	0.06	13,16,20,22	0

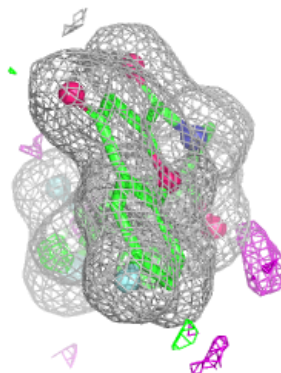
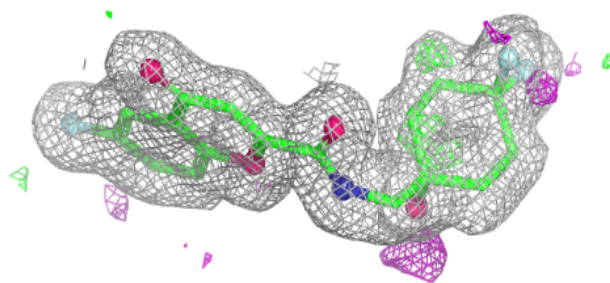
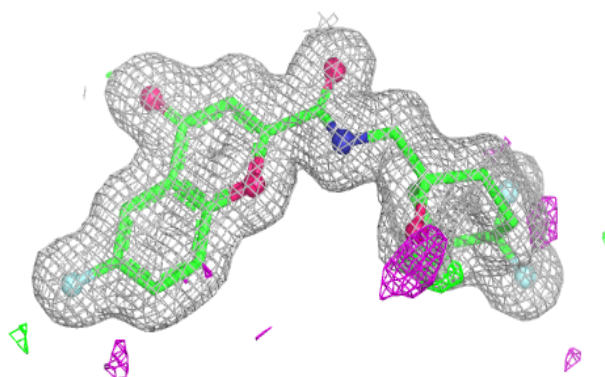
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FYB 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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.