



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 9L6E / pdb_00009l6e
Title : A novel allosteric covalent inhibitory site of fucosyltransferase 8 revealed by crystal structures
Authors : Jiang, J.; Fang, P.
Deposited on : 2024-12-24
Resolution : 3.07 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

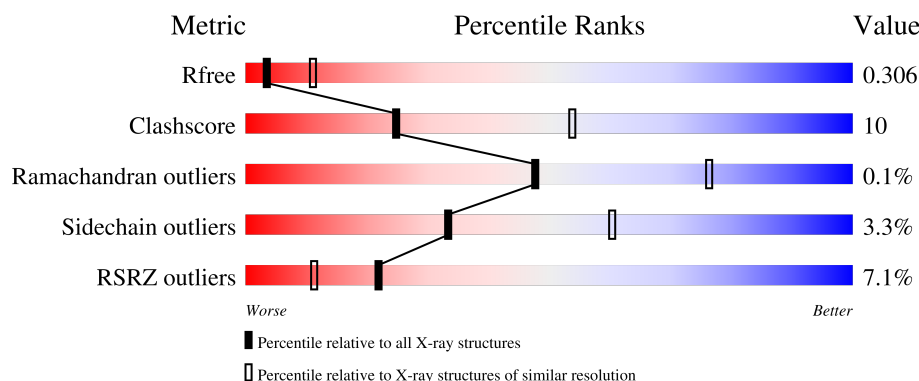
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	499	
1	B	499	

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
3	HYP	A	603	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7338 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 Alpha-(1,6)-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3647	2324	641	668	14			
1	B	442	Total	C	N	O	S	0	0	0
			3598	2292	631	661	14			

There are 56 discrepancies between the modelled and reference sequences:

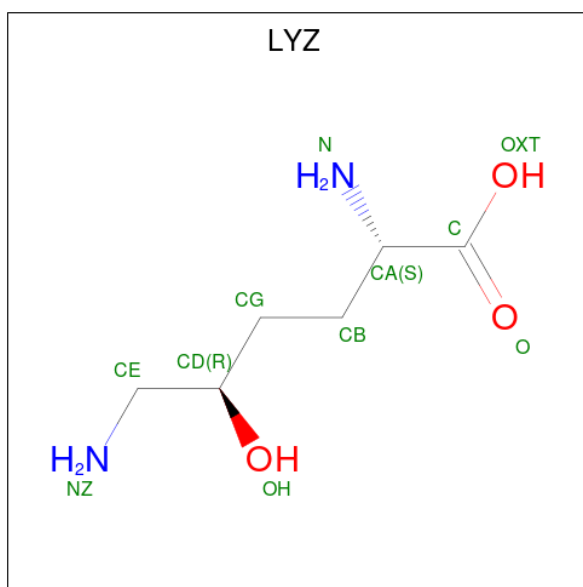
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ASP	-	expression tag	UNP Q9BYC5
A	78	ALA	-	expression tag	UNP Q9BYC5
A	79	ALA	-	expression tag	UNP Q9BYC5
A	80	GLN	-	expression tag	UNP Q9BYC5
A	81	PRO	-	expression tag	UNP Q9BYC5
A	82	ALA	-	expression tag	UNP Q9BYC5
A	83	ASP	-	expression tag	UNP Q9BYC5
A	84	TYR	-	expression tag	UNP Q9BYC5
A	85	LYS	-	expression tag	UNP Q9BYC5
A	86	ASP	-	expression tag	UNP Q9BYC5
A	87	HIS	-	expression tag	UNP Q9BYC5
A	88	ASP	-	expression tag	UNP Q9BYC5
A	89	GLY	-	expression tag	UNP Q9BYC5
A	90	ASP	-	expression tag	UNP Q9BYC5
A	91	TYR	-	expression tag	UNP Q9BYC5
A	92	LYS	-	expression tag	UNP Q9BYC5
A	93	ASP	-	expression tag	UNP Q9BYC5
A	94	HIS	-	expression tag	UNP Q9BYC5
A	95	ASP	-	expression tag	UNP Q9BYC5
A	96	ILE	-	expression tag	UNP Q9BYC5
A	97	ASP	-	expression tag	UNP Q9BYC5
A	98	TYR	-	expression tag	UNP Q9BYC5
A	99	LYS	-	expression tag	UNP Q9BYC5
A	100	ASP	-	expression tag	UNP Q9BYC5
A	101	ASP	-	expression tag	UNP Q9BYC5

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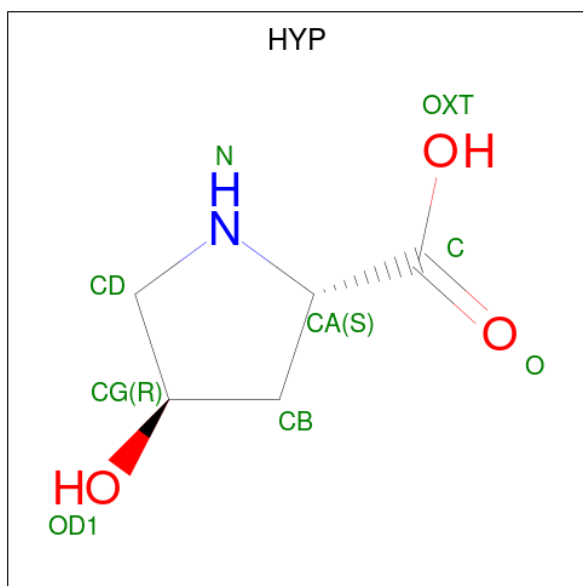
Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ASP	-	expression tag	UNP Q9BYC5
A	103	ASP	-	expression tag	UNP Q9BYC5
A	104	LYS	-	expression tag	UNP Q9BYC5
B	77	ASP	-	expression tag	UNP Q9BYC5
B	78	ALA	-	expression tag	UNP Q9BYC5
B	79	ALA	-	expression tag	UNP Q9BYC5
B	80	GLN	-	expression tag	UNP Q9BYC5
B	81	PRO	-	expression tag	UNP Q9BYC5
B	82	ALA	-	expression tag	UNP Q9BYC5
B	83	ASP	-	expression tag	UNP Q9BYC5
B	84	TYR	-	expression tag	UNP Q9BYC5
B	85	LYS	-	expression tag	UNP Q9BYC5
B	86	ASP	-	expression tag	UNP Q9BYC5
B	87	HIS	-	expression tag	UNP Q9BYC5
B	88	ASP	-	expression tag	UNP Q9BYC5
B	89	GLY	-	expression tag	UNP Q9BYC5
B	90	ASP	-	expression tag	UNP Q9BYC5
B	91	TYR	-	expression tag	UNP Q9BYC5
B	92	LYS	-	expression tag	UNP Q9BYC5
B	93	ASP	-	expression tag	UNP Q9BYC5
B	94	HIS	-	expression tag	UNP Q9BYC5
B	95	ASP	-	expression tag	UNP Q9BYC5
B	96	ILE	-	expression tag	UNP Q9BYC5
B	97	ASP	-	expression tag	UNP Q9BYC5
B	98	TYR	-	expression tag	UNP Q9BYC5
B	99	LYS	-	expression tag	UNP Q9BYC5
B	100	ASP	-	expression tag	UNP Q9BYC5
B	101	ASP	-	expression tag	UNP Q9BYC5
B	102	ASP	-	expression tag	UNP Q9BYC5
B	103	ASP	-	expression tag	UNP Q9BYC5
B	104	LYS	-	expression tag	UNP Q9BYC5

- Molecule 2 is 5-HYDROXYLYSINE (CCD ID: LYZ) (formula: $C_6H_{14}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	2	3		

- Molecule 3 is 4-HYDROXYPROLINE (CCD ID: HYP) (formula: $C_5H_9NO_3$).



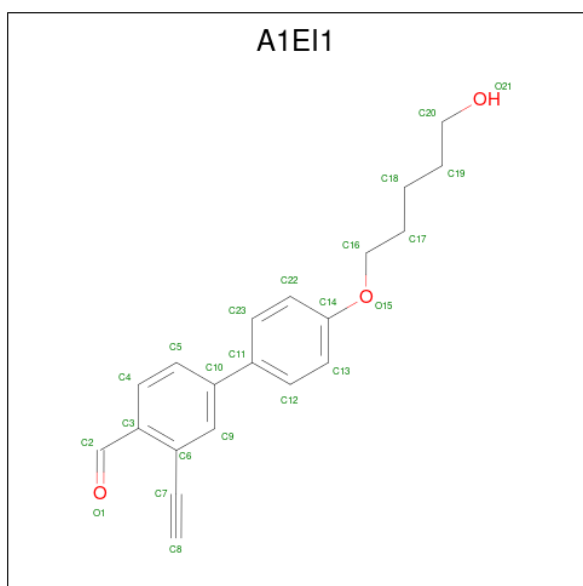
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	5	1	3		
3	A	1	Total	C	N	O	0	0
			9	5	1	3		
3	B	1	Total	C	N	O	0	0
			9	5	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			9	5	1	3		
3	B	1	Total	C	N	O	0	0
			9	5	1	3		
3	B	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 4 is 2-ethynyl-4-[4-(5-oxidanylpentoxy)phenyl]benzaldehyde (CCD ID: A1EI1) (formula: C₂₀H₂₀O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			23	20	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

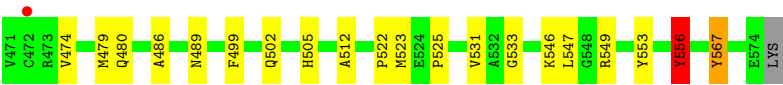
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.79Å 67.91Å 140.82Å 90.00° 132.15° 90.00°	Depositor
Resolution (Å)	71.46 – 3.07 71.46 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.3 (71.46-3.07) 99.3 (71.46-3.07)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.229 , 0.310 0.249 , 0.306	Depositor DCC
R_{free} test set	1240 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7338	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, A1EI1, HYP, LYZ, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/3741	0.67	0/5068
1	B	0.54	0/3688	0.85	4/4992 (0.1%)
All	All	0.48	0/7429	0.76	4/10060 (0.0%)

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	B	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	PRO	N-CA-CB	-5.94	97.39	103.15
1	B	556	TYR	CA-CB-CG	5.56	123.91	113.90
1	B	567	TYR	CA-CB-CG	5.35	123.54	113.90
1	B	295	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	260	ARG	Sidechain
1	B	269	ARG	Sidechain
1	B	300	ARG	Sidechain
1	B	315	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	403	ARG	Sidechain

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	3647	0	3565	77	1
1	B	3598	0	3523	77	0
2	A	11	0	13	2	0
3	A	18	0	15	4	0
3	B	36	0	32	2	0
4	B	23	0	0	0	0
5	B	2	0	0	0	0
6	B	1	0	0	0	0
7	B	2	0	0	0	0
All	All	7338	0	7148	142	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 10.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HH22	2:A:601:LYZ:HA	1.38	0.87
1:B:281:VAL:HG23	1:B:282:LYS:HE3	1.56	0.87
1:A:223:GLN:OE1	1:A:248:TRP:NE1	2.15	0.74
1:B:387:GLU:OE1	1:B:424:TYR:OH	2.05	0.74
1:B:126:LEU:HD13	1:B:159:HIS:HD2	1.52	0.73
1:A:108:LEU:HD11	1:B:176:ALA:HB1	1.71	0.71
1:B:523:MET:HE2	1:B:553:TYR:HB2	1.74	0.69
1:A:568:PRO:HB2	1:A:570:TYR:CE1	2.28	0.69
1:B:306:LEU:HD22	1:B:324:ALA:HB1	1.73	0.69
1:A:259:PHE:CZ	3:A:603:HYP:HG	2.29	0.67
1:B:556:TYR:HD1	1:B:556:TYR:C	2.02	0.66
1:B:209:LYS:HE2	1:B:266:CYS:SG	2.36	0.66
1:B:356:LYS:HB3	1:B:403:ARG:HH12	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:NZ	1:A:268:ASP:O	2.28	0.65
1:A:118:ARG:NH2	2:A:601:LYZ:HA	2.09	0.64
1:B:556:TYR:C	1:B:556:TYR:CD1	2.75	0.64
1:B:281:VAL:HG23	1:B:282:LYS:CE	2.27	0.64
1:B:350:THR:HG23	1:B:355:PHE:HB3	1.80	0.64
1:B:281:VAL:CG2	1:B:282:LYS:HE3	2.28	0.63
1:A:223:GLN:O	1:A:227:VAL:HG23	1.99	0.62
1:A:332:VAL:O	1:A:336:ILE:HG12	1.98	0.62
1:B:512:ALA:HB2	1:B:525:PRO:HD3	1.82	0.62
1:B:126:LEU:HD13	1:B:159:HIS:CD2	2.35	0.61
1:B:546:LYS:HE3	1:B:547:LEU:HD21	1.83	0.60
1:A:336:ILE:HB	3:A:603:HYP:HB2	1.83	0.60
1:A:259:PHE:HZ	3:A:603:HYP:HG	1.66	0.60
1:B:297:LEU:HD21	1:B:301:PRO:HD2	1.84	0.60
1:B:220:TYR:HD2	1:B:450:VAL:HG11	1.67	0.60
1:A:117:ARG:NH2	1:B:317:VAL:O	2.34	0.60
1:B:336:ILE:O	1:B:337:ARG:C	2.44	0.59
1:B:227:VAL:HG13	1:B:243:LEU:HD11	1.85	0.59
1:B:366:ARG:NH2	1:B:377:HIS:O	2.36	0.59
1:A:160:GLU:O	1:A:164:MET:HG2	2.04	0.58
1:A:568:PRO:HB2	1:A:570:TYR:CD1	2.38	0.58
1:A:108:LEU:HD12	1:B:179:TRP:CE3	2.40	0.57
1:A:308:VAL:HG11	1:A:323:PRO:HB2	1.87	0.56
1:A:455:HIS:HB2	3:A:603:HYP:O	2.06	0.56
1:B:305:PRO:HB3	1:B:306:LEU:HD23	1.88	0.55
1:A:214:ILE:CG2	1:A:245:SER:HA	2.38	0.54
1:A:325:VAL:HG22	1:A:497:TYR:CE2	2.43	0.54
1:A:199:GLN:O	1:A:263:SER:OG	2.20	0.54
1:B:209:LYS:HB3	1:B:242:ILE:HD13	1.90	0.54
1:A:294:VAL:HG21	1:A:501:GLY:HA3	1.89	0.52
1:A:209:LYS:HE2	1:A:266:CYS:SG	2.50	0.52
1:A:179:TRP:CE3	1:B:108:LEU:HD12	2.45	0.52
1:A:258:VAL:HG11	1:A:447:LEU:HD21	1.91	0.52
1:A:258:VAL:HG23	1:A:259:PHE:CD2	2.45	0.51
1:A:209:LYS:HB2	1:A:288:VAL:HG22	1.90	0.51
1:A:160:GLU:HG3	1:B:127:TRP:HB2	1.92	0.51
1:A:331:PHE:O	1:A:335:LEU:HG	2.11	0.51
1:A:138:LYS:O	1:B:146:GLN:NE2	2.44	0.51
1:A:383:MET:HG3	1:A:421:TYR:CE2	2.46	0.51
1:A:131:GLN:O	1:A:135:LYS:HG3	2.11	0.51
1:B:295:ASP:OD1	1:B:295:ASP:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LYS:HE3	1:A:547:LEU:HD23	1.94	0.50
1:A:233:ILE:O	1:A:237:THR:OG1	2.14	0.50
1:B:376:PHE:CD1	1:B:376:PHE:N	2.80	0.50
1:A:305:PRO:HG2	1:A:499:PHE:CD2	2.47	0.49
1:B:376:PHE:N	1:B:376:PHE:HD1	2.09	0.49
1:B:393:LEU:O	1:B:397:MET:HG2	2.12	0.49
1:A:207:ALA:O	1:A:209:LYS:HG3	2.12	0.49
1:A:417:ALA:HB1	1:A:426:PHE:CZ	2.48	0.49
1:B:259:PHE:CD1	1:B:336:ILE:HA	2.47	0.49
1:A:117:ARG:NH1	1:B:321:GLY:HA2	2.28	0.49
1:A:401:LYS:HE3	1:A:425:GLU:N	2.28	0.48
1:A:383:MET:HG3	1:A:421:TYR:HE2	1.78	0.48
1:A:445:ASN:OD1	1:A:448:ARG:NH2	2.46	0.48
1:B:214:ILE:HG22	1:B:244:GLU:O	2.14	0.48
1:B:203:ASP:OD2	1:B:205:SER:OG	2.30	0.47
1:B:204:CYS:O	1:B:209:LYS:NZ	2.46	0.47
1:A:198:LEU:HB2	1:A:570:TYR:HE2	1.79	0.47
1:B:339:GLN:HG3	1:B:341:TRP:CZ2	2.50	0.47
1:B:130:LEU:HD23	1:B:152:PHE:HZ	1.80	0.47
1:B:282:LYS:HE3	1:B:282:LYS:H	1.79	0.46
1:B:224:LEU:O	1:B:228:VAL:HG23	2.16	0.46
1:A:568:PRO:HB2	1:A:570:TYR:HE1	1.74	0.46
1:A:473:ARG:NH1	1:A:498:TYR:CE2	2.84	0.46
1:A:210:LEU:HD12	1:A:239:ARG:HD2	1.97	0.45
1:B:261:PRO:C	1:B:263:SER:H	2.25	0.45
1:A:205:SER:O	1:A:287:GLN:NE2	2.46	0.45
1:B:199:GLN:HA	1:B:240:THR:HG23	1.98	0.45
1:A:403:ARG:HG2	1:A:425:GLU:HB3	1.97	0.45
1:A:218:CYS:HB3	1:A:222:CYS:HB2	1.53	0.45
1:B:480:GLN:HE22	1:B:486:ALA:C	2.24	0.45
1:B:126:LEU:HB2	1:B:159:HIS:CD2	2.52	0.45
1:B:405:TYR:OH	1:B:453:ASP:OD1	2.13	0.45
1:A:408:THR:HG21	1:A:413:LEU:HD23	1.99	0.45
1:B:360:ILE:O	1:B:404:VAL:HA	2.17	0.44
1:A:120:GLU:HA	1:B:167:LEU:HD13	1.99	0.44
1:A:230:CYS:HA	1:A:291:LEU:CD2	2.47	0.44
1:B:233:ILE:HD12	1:B:291:LEU:HD21	2.00	0.44
1:B:522:PRO:HD3	1:B:549:ARG:NH1	2.32	0.44
1:A:468:SER:HA	1:A:498:TYR:OH	2.18	0.44
1:B:359:VAL:HG23	1:B:403:ARG:HB3	2.00	0.44
1:A:556:TYR:CG	1:B:159:HIS:ND1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ALA:O	1:B:317:VAL:HG23	2.18	0.43
1:A:546:LYS:HE2	1:A:546:LYS:HB3	1.69	0.43
1:B:505:HIS:O	1:B:531:VAL:HG12	2.18	0.43
1:A:244:GLU:OE2	1:A:269:ARG:HD2	2.19	0.43
1:B:179:TRP:HZ2	1:B:318:ARG:HH21	1.65	0.43
1:A:118:ARG:HD2	1:A:166:ASP:OD2	2.19	0.43
1:B:281:VAL:CG2	1:B:282:LYS:CE	2.94	0.43
1:B:356:LYS:HB3	1:B:403:ARG:NH1	2.30	0.43
1:A:360:ILE:HD12	1:A:390:PHE:CE2	2.54	0.43
1:B:305:PRO:HG2	1:B:499:PHE:CD2	2.54	0.43
1:B:126:LEU:HB2	1:B:159:HIS:NE2	2.34	0.42
1:B:306:LEU:HG	1:B:502:GLN:OE1	2.19	0.42
1:B:470:GLN:O	1:B:474:VAL:HG23	2.19	0.42
1:A:326:TRP:O	1:A:329:SER:OG	2.30	0.42
1:B:223:GLN:O	1:B:226:HIS:HB3	2.20	0.42
1:B:336:ILE:O	1:B:338:PRO:N	2.52	0.42
1:A:214:ILE:HG22	1:A:245:SER:HA	2.02	0.42
1:A:255:TRP:HZ2	1:A:335:LEU:HB3	1.84	0.42
1:B:257:THR:HG22	3:B:604:HYP:HB2	2.01	0.42
1:A:334:TYR:O	1:A:337:ARG:NE	2.37	0.42
1:B:126:LEU:HD11	1:B:156:LEU:HD22	2.02	0.42
1:B:253:GLY:C	1:B:255:TRP:H	2.27	0.42
1:A:170:LEU:HD12	1:A:170:LEU:HA	1.85	0.42
1:B:160:GLU:O	1:B:164:MET:HG2	2.20	0.42
1:A:316:LEU:O	1:A:320:HIS:N	2.52	0.41
1:B:533:GLY:HA3	3:B:602:HYP:HA	2.01	0.41
1:B:198:LEU:HD22	1:B:235:TYR:HA	2.02	0.41
1:A:261:PRO:HB2	1:A:263:SER:O	2.20	0.41
1:B:297:LEU:HD21	1:B:301:PRO:CD	2.50	0.41
1:B:455:HIS:O	1:B:458:SER:OG	2.27	0.41
1:B:479:MET:HE3	1:B:489:ASN:HB2	2.02	0.41
1:A:467:PHE:O	1:A:473:ARG:HD3	2.21	0.41
1:B:152:PHE:O	1:B:156:LEU:HG	2.20	0.41
1:A:167:LEU:HD13	1:B:120:GLU:HA	2.03	0.41
1:A:210:LEU:HD21	1:A:291:LEU:HD22	2.02	0.41
1:A:259:PHE:O	1:A:339:GLN:HG2	2.21	0.41
1:A:159:HIS:CG	1:B:556:TYR:CD2	3.08	0.41
1:A:214:ILE:HG21	1:A:245:SER:HA	2.01	0.41
1:A:505:HIS:O	1:A:531:VAL:HG12	2.21	0.41
1:A:180:ARG:HG3	1:A:319:VAL:HG23	2.02	0.40
1:A:260:ARG:HB3	1:A:261:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ILE:HD13	1:A:478:ILE:HG21	1.92	0.40
1:A:556:TYR:HB3	1:B:159:HIS:CE1	2.56	0.40
1:A:383:MET:HE1	1:A:404:VAL:HG21	2.04	0.40
1:A:229:TYR:OH	1:A:297:LEU:HD22	2.20	0.40
1:B:429:ASP:OD2	1:B:449:GLY:HA2	2.22	0.40
1:A:377:HIS:HB2	1:A:382:TYR:HE1	1.86	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)
1:A:545:ARG:O	1:A:545:ARG:O[2_556]	1.84	0.36

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	441/499 (88%)	418 (95%)	23 (5%)	0	100	100
1	B	434/499 (87%)	414 (95%)	19 (4%)	1 (0%)	43	71
All	All	875/998 (88%)	832 (95%)	42 (5%)	1 (0%)	48	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	VAL

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	394/437 (90%)	386 (98%)	8 (2%)	48	69
1	B	391/437 (90%)	373 (95%)	18 (5%)	24	53
All	All	785/874 (90%)	759 (97%)	26 (3%)	33	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	ARG
1	A	310	GLU
1	A	311	ASP
1	A	315	ARG
1	A	382	TYR
1	A	543	VAL
1	A	546	LYS
1	A	547	LEU
1	B	260	ARG
1	B	268	ASP
1	B	272	ILE
1	B	281	VAL
1	B	282	LYS
1	B	295	ASP
1	B	308	VAL
1	B	311	ASP
1	B	314	ASP
1	B	315	ARG
1	B	325	VAL
1	B	376	PHE
1	B	382	TYR
1	B	396	ARG
1	B	467	PHE
1	B	469	SER
1	B	556	TYR
1	B	567	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	HIS

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Mol	Chain	Res	Type
1	A	398	GLN
1	B	213	ASN
1	B	226	HIS
1	B	330	GLN
1	B	357	HIS
1	B	389	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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$
3	HYP	B	602	-	9,9,9	1.64	3 (33%)	10,12,12	1.60	2 (20%)
3	HYP	A	602	-	9,9,9	1.31	1 (11%)	10,12,12	1.34	1 (10%)
2	LYZ	A	601	-	8,10,10	0.92	0	6,12,12	1.80	1 (16%)
4	A1EI1	B	601	-	24,24,24	0.38	0	30,30,30	0.36	0
3	HYP	A	603	-	9,9,9	1.44	1 (11%)	10,12,12	1.64	3 (30%)
3	HYP	B	604	-	9,9,9	1.56	2 (22%)	10,12,12	1.77	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HYP	B	603	-	9,9,9	1.25	1 (11%)	10,12,12	1.23	1 (10%)
3	HYP	B	605	-	9,9,9	1.64	2 (22%)	10,12,12	1.60	3 (30%)

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
3	HYP	B	602	-	-	4/4/13/13	0/1/1/1
3	HYP	A	602	-	-	0/4/13/13	0/1/1/1
2	LYZ	A	601	-	-	3/11/11/11	-
4	A1EI1	B	601	-	-	4/14/15/15	0/2/2/2
3	HYP	A	603	-	-	0/4/13/13	0/1/1/1
3	HYP	B	604	-	-	2/4/13/13	0/1/1/1
3	HYP	B	603	-	-	4/4/13/13	0/1/1/1
3	HYP	B	605	-	-	4/4/13/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	605	HYP	CA-C	3.51	1.61	1.52
3	B	602	HYP	CD-CG	2.84	1.59	1.53
3	B	604	HYP	CA-C	2.82	1.59	1.52
3	A	602	HYP	CB-CG	2.63	1.57	1.52
3	A	603	HYP	CD-CG	2.53	1.59	1.53
3	B	602	HYP	CA-C	2.51	1.59	1.52
3	B	605	HYP	CD-CG	2.30	1.58	1.53
3	B	604	HYP	CD-CG	2.28	1.58	1.53
3	B	603	HYP	CD-CG	2.26	1.58	1.53
3	B	602	HYP	CB-CG	2.20	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	LYZ	OXT-C-O	-3.88	115.27	124.08
3	B	604	HYP	CG-CB-CA	3.84	108.19	103.75
3	A	603	HYP	OD1-CG-CD	3.37	117.18	110.30
3	B	602	HYP	OD1-CG-CD	3.15	116.74	110.30
3	A	602	HYP	OD1-CG-CB	3.00	117.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	HYP	OD1-CG-CB	2.70	116.67	110.10
3	B	602	HYP	OD1-CG-CB	2.69	116.63	110.10
3	B	605	HYP	CG-CB-CA	2.67	106.84	103.75
3	B	603	HYP	OD1-CG-CB	2.66	116.55	110.10
3	B	605	HYP	OD1-CG-CB	2.54	116.26	110.10
3	B	605	HYP	OD1-CG-CD	2.45	115.31	110.30
3	B	604	HYP	OD1-CG-CD	2.37	115.15	110.30
3	B	604	HYP	OD1-CG-CB	2.34	115.78	110.10
3	A	603	HYP	C-CA-N	2.19	115.39	106.84

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	HYP	O-C-CA-N
3	B	602	HYP	OXT-C-CA-N
3	B	602	HYP	O-C-CA-CB
3	B	602	HYP	OXT-C-CA-CB
3	B	603	HYP	O-C-CA-N
3	B	603	HYP	OXT-C-CA-N
3	B	603	HYP	O-C-CA-CB
3	B	603	HYP	OXT-C-CA-CB
3	B	605	HYP	O-C-CA-N
3	B	605	HYP	OXT-C-CA-N
3	B	605	HYP	O-C-CA-CB
3	B	605	HYP	OXT-C-CA-CB
2	A	601	LYZ	OH-CD-CG-CB
4	B	601	A1EI1	C5-C10-C11-C23
4	B	601	A1EI1	C5-C10-C11-C12
2	A	601	LYZ	CA-CB-CG-CD
4	B	601	A1EI1	C9-C10-C11-C12
4	B	601	A1EI1	C9-C10-C11-C23
2	A	601	LYZ	CE-CD-CG-CB
3	B	604	HYP	O-C-CA-CB
3	B	604	HYP	OXT-C-CA-CB

There are no ring outliers.

4 monomers are involved in 8 short contacts:

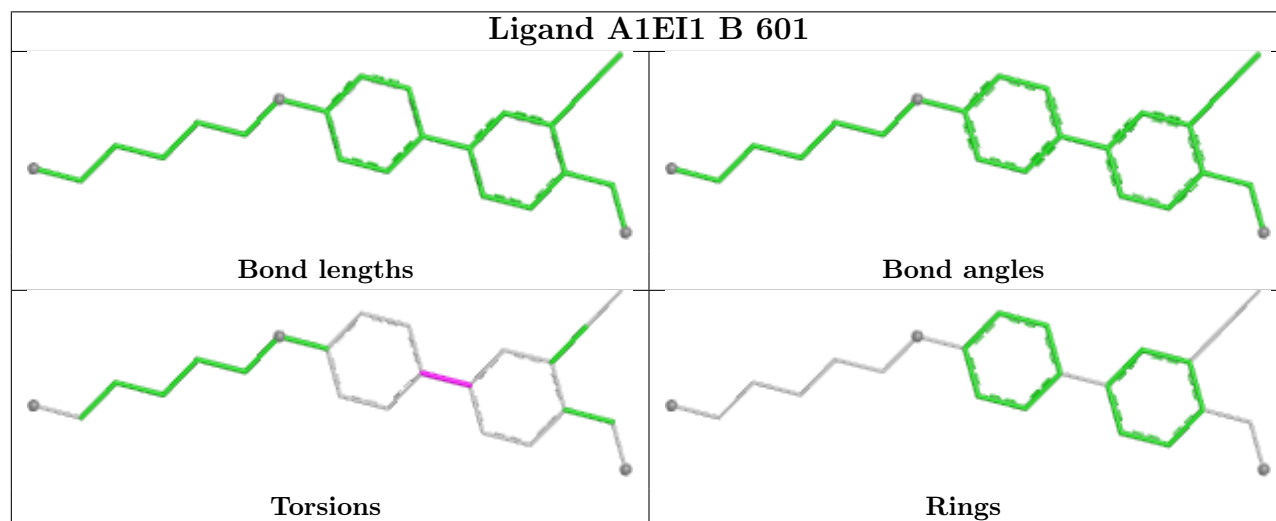
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	HYP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	LYZ	2	0
3	A	603	HYP	4	0
3	B	604	HYP	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 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	447/499 (89%)	0.89	34 (7%)	20 10	56, 72, 107, 136	0
1	B	442/499 (88%)	0.66	29 (6%)	24 12	46, 64, 89, 118	0
All	All	889/998 (89%)	0.78	63 (7%)	22 11	46, 67, 102, 136	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	CYS	5.1
1	B	266	CYS	4.0
1	B	222	CYS	3.4
1	B	204	CYS	3.3
1	A	428	SER	3.3
1	B	432	ILE	3.3
1	B	301	PRO	3.2
1	B	472	CYS	3.2
1	B	446	SER	3.2
1	B	376	PHE	3.1
1	B	148	HIS	3.0
1	A	274	THR	2.9
1	B	178	ASP	2.8
1	A	215	ASN	2.8
1	A	250	TYR	2.8
1	B	433	SER	2.7
1	B	298	HIS	2.7
1	B	268	ASP	2.6
1	B	423	ASN	2.6
1	A	181	GLU	2.6
1	A	204	CYS	2.6
1	A	222	CYS	2.5
1	A	572	GLU	2.5
1	A	251	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	174	ASP	2.5
1	A	213	ASN	2.5
1	B	445	ASN	2.4
1	A	218	CYS	2.4
1	A	465	CYS	2.4
1	A	375	ALA	2.4
1	A	245	SER	2.4
1	B	218	CYS	2.4
1	A	314	ASP	2.4
1	A	246	GLN	2.4
1	A	247	ASN	2.3
1	A	248	TRP	2.3
1	A	252	THR	2.3
1	B	230	CYS	2.3
1	A	430	ASN	2.2
1	B	264	GLU	2.2
1	A	479	MET	2.2
1	B	253	GLY	2.2
1	B	383	MET	2.2
1	A	150	ASP	2.2
1	A	409	ASP	2.2
1	B	311	ASP	2.2
1	B	419	THR	2.1
1	A	232	MET	2.1
1	A	523	MET	2.1
1	A	253	GLY	2.1
1	A	272	ILE	2.1
1	A	377	HIS	2.1
1	A	279	GLY	2.1
1	B	142	GLY	2.1
1	B	217	GLY	2.1
1	B	280	GLU	2.1
1	B	202	LYS	2.0
1	A	257	THR	2.0
1	A	311	ASP	2.0
1	B	189	GLU	2.0
1	B	245	SER	2.0
1	B	279	GLY	2.0
1	A	214	ILE	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](#)

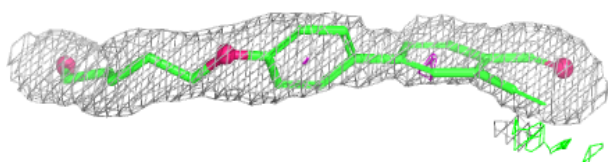
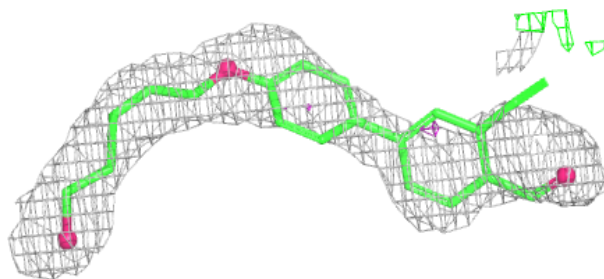
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	HYP	B	603	9/9	0.77	0.22	66,71,84,87	0
3	HYP	A	603	9/9	0.78	0.19	77,77,90,91	0
3	HYP	B	605	9/9	0.79	0.15	65,73,81,83	0
3	HYP	A	602	9/9	0.80	0.24	63,70,80,83	0
3	HYP	B	604	9/9	0.82	0.20	73,79,86,87	0
6	NA	B	608	1/1	0.82	0.10	24,24,24,24	0
2	LYZ	A	601	11/11	0.83	0.17	62,72,83,85	0
4	A1EI1	B	601	23/23	0.83	0.21	59,80,91,97	0
3	HYP	B	602	9/9	0.83	0.19	67,69,77,80	0
5	CL	B	607	1/1	0.88	0.32	30,30,30,30	0
5	CL	B	606	1/1	0.90	0.08	45,45,45,45	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 A1EI1 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.