



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:59 PM UTC

PDB ID : 9B25 / pdb\_00009b25  
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with NA98  
Authors : Nwachukwu, J.C.; Min, C.K.; Papa, A.; Rangarajan, E.S.; Izard, T.; Sharma, A.; Nettles, K.W.  
Deposited on : 2024-03-14  
Resolution : 1.45 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

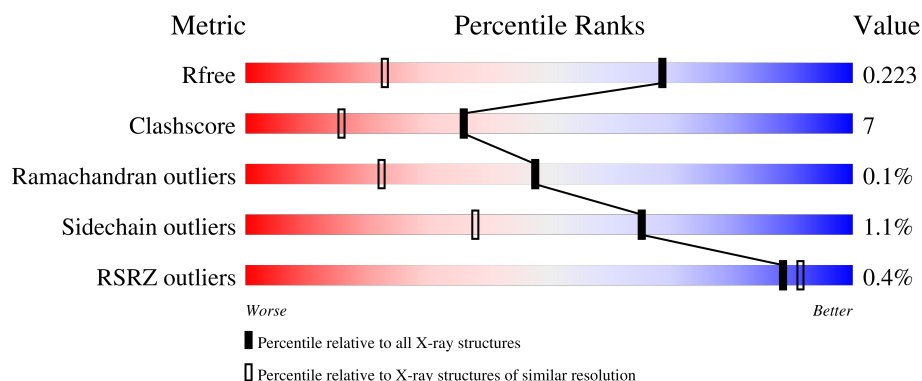
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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  $\geq 3$ , 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	251	 84% 15%
1	B	251	 82% 10% • 7%
1	C	251	 86% 13%
1	D	251	 80% 14% 6%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16412 atoms, of which 7941 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 Estrogen receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	250	Total	C	H	N	O	S	0	4	0
			4052	1277	2048	344	364	19			
1	B	233	Total	C	H	N	O	S	0	0	0
			3683	1172	1849	313	330	19			
1	C	250	Total	C	H	N	O	S	0	4	0
			4032	1269	2038	345	361	19			
1	D	236	Total	C	H	N	O	S	0	1	0
			3747	1192	1878	318	340	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	ALA	-	expression tag	UNP P03372
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	297	ALA	-	expression tag	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	297	ALA	-	expression tag	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	297	ALA	-	expression tag	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is (1r,4r)-N-[4-(4-{[6-hydroxy-2-(4-hydroxyphenyl)-1-benzothiophen-3-yl]oxy}phenoxy)butyl]-4-(trifluoromethyl)cyclohexane-1-carboxamide (CCD ID: A1AIZ) (formula: C<sub>32</sub>H<sub>32</sub>F<sub>3</sub>NO<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



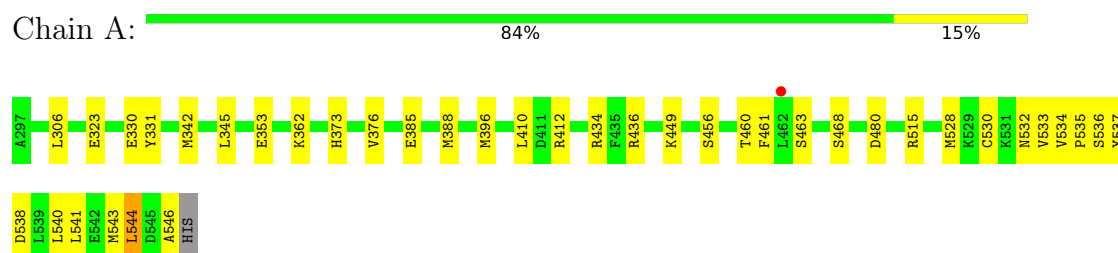
- Molecule 3 is water.



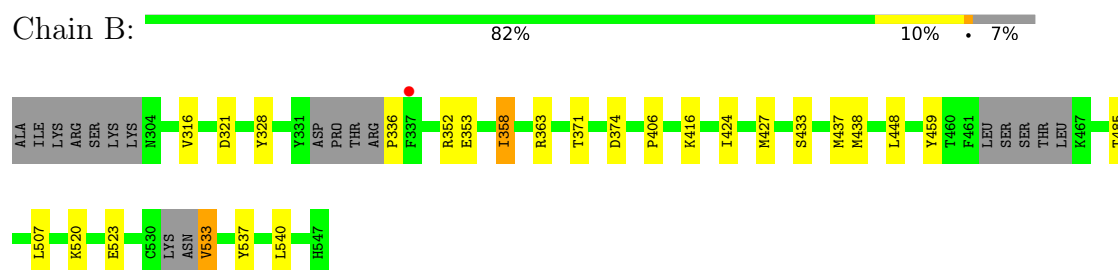
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

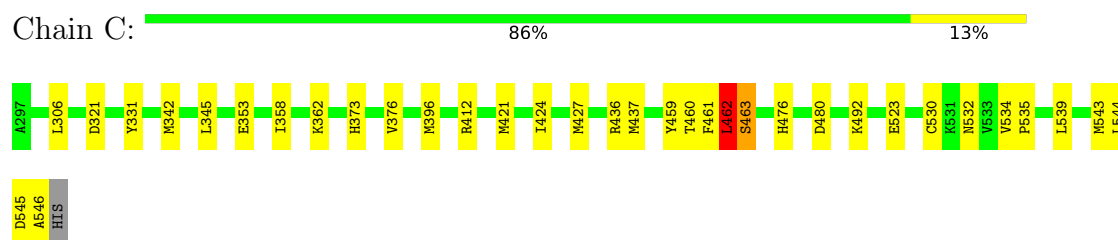
#### • Molecule 1: Estrogen receptor



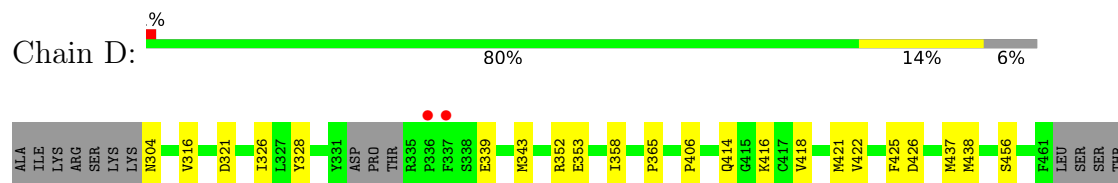
#### • Molecule 1: Estrogen receptor



#### • Molecule 1: Estrogen receptor



#### • Molecule 1: Estrogen receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.83Å 199.98Å 55.25Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	48.29 – 1.45 48.29 – 1.45	Depositor EDS
% Data completeness (in resolution range)	69.9 (48.29-1.45) 69.7 (48.29-1.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.194 , 0.223 0.194 , 0.223	Depositor DCC
$R_{free}$ test set	6197 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h-l,k,h 0.011 for l,k,-h-l 0.477 for h,-k,-h-l 0.019 for -h-l,-k,l 0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YCM, A1AIZ

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	0.54	0/2049	0.62	1/2767 (0.0%)
1	B	0.37	0/1855	0.49	0/2503
1	C	0.57	1/2038 (0.0%)	0.74	5/2751 (0.2%)
1	D	0.37	0/1891	0.47	0/2555
All	All	0.48	1/7833 (0.0%)	0.59	6/10576 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	463	SER	CA-C	-5.21	1.45	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	461	PHE	N-CA-C	-13.21	96.88	111.14
1	C	463	SER	N-CA-C	7.19	126.11	110.80
1	C	462	LEU	CA-C-N	6.29	133.56	121.54
1	C	462	LEU	C-N-CA	6.29	133.56	121.54
1	C	462	LEU	CB-CG-CD2	-5.79	93.33	110.70
1	A	388	MET	N-CA-CB	-5.02	102.74	110.12

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	336	PRO	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	2004	2048	2026	35	0
1	B	1834	1849	1848	24	0
1	C	1994	2038	2017	34	0
1	D	1869	1878	1875	28	0
2	A	42	32	0	4	0
2	B	42	32	0	1	0
2	C	42	32	0	1	0
2	D	42	32	0	1	0
3	A	192	0	0	19	1
3	B	114	0	0	8	0
3	C	192	0	0	10	1
3	D	104	0	0	7	0
All	All	8471	7941	7766	114	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 (114) 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:C:530:CYS:SG	3:C:873:HOH:O	2.07	1.12
1:A:530:CYS:SG	3:A:874:HOH:O	2.11	1.08
1:A:434:ARG:NE	3:A:701:HOH:O	1.86	1.06
1:D:437:MET:SD	3:D:793:HOH:O	2.13	1.05
1:A:543:MET:HE3	1:C:544:LEU:HD13	1.39	1.02
1:A:536:SER:HB3	3:A:706:HOH:O	1.57	1.01
1:C:342:MET:HE2	1:C:421:MET:HE1	1.41	0.99
1:A:385:GLU:OE1	3:A:702:HOH:O	1.86	0.91
1:D:304:ASN:O	3:D:701:HOH:O	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:MET:CE	1:C:544:LEU:HD13	2.07	0.84
1:A:330:GLU:OE2	3:A:703:HOH:O	1.96	0.83
1:D:343:MET:HE2	1:D:528:MET:SD	2.18	0.83
1:C:373:HIS:NE2	3:C:701:HOH:O	2.01	0.81
1:A:480:ASP:OD2	3:A:705:HOH:O	1.99	0.80
1:B:520:LYS:NZ	3:B:701:HOH:O	1.98	0.78
1:A:373:HIS:NE2	3:A:704:HOH:O	1.97	0.77
1:B:416:LYS:NZ	3:B:702:HOH:O	2.15	0.77
1:C:480:ASP:OD2	3:C:702:HOH:O	2.01	0.77
1:C:342:MET:CE	1:C:421:MET:HE1	2.15	0.77
1:B:328:TYR:O	1:B:352:ARG:NH2	2.20	0.73
1:A:543:MET:HE3	1:C:544:LEU:CD1	2.19	0.72
1:D:438:MET:HE1	1:D:507:LEU:HD23	1.72	0.71
1:D:414:GLN:OE1	3:D:702:HOH:O	2.08	0.71
1:D:328:TYR:O	1:D:352:ARG:NH2	2.24	0.67
3:A:701:HOH:O	1:B:459:TYR:CE1	2.47	0.67
1:A:538:ASP:OD1	3:A:706:HOH:O	2.12	0.66
1:B:363:ARG:NH2	3:B:704:HOH:O	2.20	0.66
1:B:358:ILE:CD1	1:B:540:LEU:HD22	2.26	0.65
1:B:433:SER:O	1:B:437:MET:HG3	1.97	0.64
1:D:438:MET:HE1	1:D:507:LEU:CD2	2.29	0.63
1:D:520:LYS:HA	1:D:520:LYS:HE2	1.81	0.62
1:A:543:MET:CE	1:C:544:LEU:CD1	2.76	0.61
1:A:460:THR:N	3:A:710:HOH:O	2.31	0.61
1:C:306:LEU:HD21	3:C:881:HOH:O	2.01	0.60
1:D:437:MET:CE	3:D:793:HOH:O	2.48	0.59
3:A:701:HOH:O	1:B:459:TYR:HE1	1.85	0.58
1:B:363:ARG:NE	3:B:704:HOH:O	2.31	0.57
1:C:476:HIS:NE2	3:C:702:HOH:O	2.32	0.57
1:A:434:ARG:CZ	3:A:701:HOH:O	2.38	0.56
1:B:358:ILE:HD13	1:B:540:LEU:HD22	1.87	0.56
1:D:437:MET:HA	1:D:437:MET:HE3	1.88	0.56
1:A:528:MET:HB3	1:A:533:VAL:HG23	1.88	0.55
1:C:545:ASP:O	1:C:546:ALA:HB2	2.05	0.55
1:B:424:ILE:HA	1:B:427:MET:HE2	1.89	0.55
1:B:523:GLU:OE1	3:B:701:HOH:O	2.19	0.52
1:D:421:MET:HE3	1:D:425:PHE:CZ	2.44	0.52
1:C:321:ASP:OD2	3:C:703:HOH:O	2.19	0.52
1:A:331:TYR:CB	1:A:345:LEU:HD21	2.41	0.51
1:C:460:THR:N	3:C:711:HOH:O	2.42	0.51
1:B:358:ILE:HD12	1:B:540:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ARG:NE	3:C:709:HOH:O	2.39	0.50
1:A:541:LEU:HD21	3:A:790:HOH:O	2.11	0.50
1:A:540:LEU:HD23	2:A:600:A1AIZ:C16	2.41	0.50
1:B:321:ASP:OD1	3:B:703:HOH:O	2.19	0.50
1:C:534:VAL:HG13	1:C:535:PRO:HD2	1.94	0.50
1:C:436:ARG:CD	3:C:709:HOH:O	2.60	0.49
1:C:459:TYR:HB2	3:C:711:HOH:O	2.12	0.49
1:A:376:VAL:CG1	1:A:544:LEU:HD11	2.43	0.49
1:A:537:TYR:HE2	2:A:600:A1AIZ:C23	2.25	0.49
1:D:328:TYR:CE2	1:D:406:PRO:HB2	2.48	0.49
1:B:448:LEU:HD11	1:B:507:LEU:HD22	1.95	0.48
1:A:362:LYS:HE2	3:A:728:HOH:O	2.13	0.48
1:A:540:LEU:HD23	2:A:600:A1AIZ:C09	2.44	0.48
1:B:363:ARG:CZ	3:B:704:HOH:O	2.60	0.48
1:D:365:PRO:HA	3:D:791:HOH:O	2.14	0.47
1:C:331:TYR:HB2	1:C:345:LEU:HD21	1.96	0.47
1:C:539:LEU:O	1:C:543:MET:HG3	2.14	0.47
1:A:306:LEU:HD21	3:A:877:HOH:O	2.14	0.47
1:B:328:TYR:CE1	1:B:406:PRO:HB2	2.49	0.47
1:A:515:ARG:CD	3:A:702:HOH:O	2.62	0.47
1:A:331:TYR:HB3	1:A:345:LEU:CD2	2.45	0.46
1:C:523:GLU:OE1	1:D:523:GLU:OE2	2.33	0.46
1:D:326:ILE:HD11	1:D:406:PRO:HD3	1.98	0.46
1:D:539:LEU:O	1:D:543:MET:HG3	2.16	0.46
1:A:323:GLU:OE1	1:A:449:LYS:NZ	2.42	0.46
1:B:358:ILE:HD13	1:B:540:LEU:HB3	1.98	0.46
1:B:321:ASP:OD2	3:B:705:HOH:O	2.21	0.45
1:D:456:SER:HA	1:D:515:ARG:NH2	2.31	0.45
1:D:321:ASP:HB2	3:D:718:HOH:O	2.15	0.45
1:B:438:MET:HE1	1:B:507:LEU:CD2	2.46	0.45
3:A:711:HOH:O	1:C:532:ASN:HB3	2.16	0.45
1:A:353:GLU:OE2	2:A:600:A1AIZ:O05	2.35	0.45
1:A:463:SER:HA	1:A:468:SER:OG	2.17	0.45
3:A:711:HOH:O	1:C:532:ASN:CB	2.64	0.45
1:A:342:MET:HE3	1:A:410:LEU:HD13	1.99	0.44
1:A:331:TYR:HB2	1:A:345:LEU:HD21	1.99	0.44
1:A:456:SER:HA	1:A:515:ARG:NH2	2.32	0.44
1:C:331:TYR:HB3	1:C:345:LEU:CD2	2.47	0.44
1:C:353:GLU:OE2	2:C:600:A1AIZ:O05	2.36	0.44
1:D:353:GLU:OE2	2:D:600:A1AIZ:O05	2.36	0.44
1:A:534:VAL:HG13	1:A:535:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:TYR:CB	1:C:345:LEU:HD21	2.48	0.43
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.53	0.43
1:C:492:LYS:HB3	1:C:492:LYS:NZ	2.33	0.43
1:D:316:VAL:HG23	1:D:485:THR:HG23	2.00	0.43
1:B:353:GLU:OE2	2:B:600:A1AIZ:O05	2.37	0.42
1:A:396:MET:O	1:A:436:ARG:HD3	2.19	0.42
1:A:546:ALA:HB3	1:C:376:VAL:HG21	2.02	0.42
1:B:316:VAL:HG23	1:B:485:THR:CG2	2.50	0.42
1:C:545:ASP:O	1:C:546:ALA:CB	2.64	0.42
1:C:358:ILE:HG22	1:C:362:LYS:HE2	2.01	0.42
1:D:526:TYR:CD1	1:D:526:TYR:C	2.97	0.42
1:B:371:THR:HG23	1:B:374:ASP:H	1.84	0.41
1:C:437:MET:HA	1:C:437:MET:HE2	2.01	0.41
1:C:462:LEU:HD21	1:D:426:ASP:HB3	2.01	0.41
1:B:533:VAL:HG13	1:B:537:TYR:HB2	2.01	0.41
1:C:396:MET:O	1:C:436:ARG:HD3	2.20	0.41
1:D:518:SER:O	1:D:522:MET:HG2	2.21	0.41
1:D:416:LYS:CG	1:D:422:VAL:HG11	2.51	0.41
1:D:437:MET:HE1	3:D:793:HOH:O	2.18	0.40
1:A:306:LEU:HG	3:A:758:HOH:O	2.21	0.40
1:C:424:ILE:HA	1:C:427:MET:HE3	2.04	0.40
1:D:339:GLU:OE1	1:D:418:VAL:HA	2.21	0.40
1:D:358:ILE:HG21	1:D:543:MET:HB2	2.03	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)
3:A:844:HOH:O	3:C:844:HOH:O[1_554]	2.14	0.06

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/251 (100%)	249 (99%)	2 (1%)	0	100	100
1	B	224/251 (89%)	221 (99%)	3 (1%)	0	100	100
1	C	251/251 (100%)	248 (99%)	2 (1%)	1 (0%)	30	11
1	D	230/251 (92%)	224 (97%)	6 (3%)	0	100	100
All	All	956/1004 (95%)	942 (98%)	13 (1%)	1 (0%)	48	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	463	SER

### 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	226/225 (100%)	222 (98%)	4 (2%)	51	19
1	B	202/225 (90%)	200 (99%)	2 (1%)	68	42
1	C	224/225 (100%)	222 (99%)	2 (1%)	70	46
1	D	206/225 (92%)	205 (100%)	1 (0%)	81	64
All	All	858/900 (95%)	849 (99%)	9 (1%)	65	42

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	ARG
1	A	461	PHE
1	A	532	ASN
1	A	544	LEU
1	B	358	ILE
1	B	533	VAL
1	C	412	ARG
1	C	462	LEU
1	D	530	CYS

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

Mol	Chain	Res	Type
1	B	359	ASN
1	B	476	HIS
1	D	348	ASN
1	D	359	ASN
1	D	441	GLN
1	D	488	HIS
1	D	519	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	YCM	D	381	1	7,9,10	0.96	0	5,10,12	0.34	0
1	YCM	A	381	1	7,9,10	1.13	0	5,10,12	0.79	0
1	YCM	C	381	1	7,9,10	1.12	0	5,10,12	1.04	0
1	YCM	B	381	1	7,9,10	1.09	0	5,10,12	0.55	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
1	YCM	D	381	1	-	1/6/8/10	-
1	YCM	A	381	1	-	1/6/8/10	-
1	YCM	C	381	1	-	1/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	B	381	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381	YCM	SG-CD-CE-NZ2
1	C	381	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-NZ2
1	B	381	YCM	CE-CD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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$
2	A1AIZ	D	600	-	45,46,46	3.49	16 (35%)	63,65,65	2.08	22 (34%)
2	A1AIZ	C	600	-	45,46,46	3.10	14 (31%)	63,65,65	2.36	23 (36%)
2	A1AIZ	A	600	-	45,46,46	3.14	16 (35%)	63,65,65	2.11	18 (28%)
2	A1AIZ	B	600	-	45,46,46	3.59	17 (37%)	63,65,65	2.21	21 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1AIZ	D	600	-	-	2/27/37/37	0/5/5/5
2	A1AIZ	C	600	-	-	13/27/37/37	0/5/5/5
2	A1AIZ	A	600	-	-	3/27/37/37	0/5/5/5
2	A1AIZ	B	600	-	-	3/27/37/37	0/5/5/5

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	A1AIZ	C02-S01	-17.29	1.53	1.74
2	D	600	A1AIZ	C02-S01	-16.69	1.54	1.74
2	A	600	A1AIZ	C02-S01	-14.58	1.56	1.74
2	C	600	A1AIZ	C02-S01	-13.38	1.58	1.74
2	B	600	A1AIZ	C15-S01	-10.37	1.53	1.74
2	D	600	A1AIZ	C15-S01	-9.94	1.54	1.74
2	C	600	A1AIZ	C15-S01	-9.69	1.55	1.74
2	A	600	A1AIZ	C15-S01	-9.43	1.55	1.74
2	B	600	A1AIZ	C07-C02	-5.72	1.36	1.48
2	D	600	A1AIZ	C07-C02	-5.49	1.36	1.48
2	D	600	A1AIZ	C28-C04	-4.74	1.34	1.45
2	B	600	A1AIZ	C28-C04	-4.59	1.34	1.45
2	C	600	A1AIZ	C28-C04	-4.57	1.34	1.45
2	C	600	A1AIZ	C07-C02	-4.30	1.39	1.48
2	A	600	A1AIZ	C07-C02	-4.16	1.39	1.48
2	B	600	A1AIZ	C28-C15	-4.13	1.35	1.41
2	A	600	A1AIZ	C28-C04	-4.10	1.35	1.45
2	D	600	A1AIZ	C28-C15	-4.05	1.35	1.41
2	C	600	A1AIZ	C28-C15	-3.98	1.35	1.41
2	C	600	A1AIZ	C18-C03	-3.38	1.33	1.38
2	A	600	A1AIZ	C10-C07	-3.38	1.34	1.39
2	A	600	A1AIZ	C13-C12	-3.28	1.32	1.39
2	C	600	A1AIZ	C10-C07	-3.22	1.34	1.39
2	A	600	A1AIZ	C28-C15	-3.20	1.36	1.41
2	B	600	A1AIZ	C14-C07	-3.14	1.34	1.39
2	C	600	A1AIZ	C29-C28	-3.14	1.35	1.39
2	C	600	A1AIZ	C11-C10	-3.09	1.33	1.38
2	C	600	A1AIZ	C13-C12	-2.98	1.33	1.39
2	D	600	A1AIZ	C11-C10	-2.84	1.34	1.38
2	B	600	A1AIZ	C11-C10	-2.82	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	A1AIZ	C14-C07	-2.82	1.35	1.39
2	B	600	A1AIZ	C30-C29	-2.80	1.34	1.38
2	B	600	A1AIZ	C21-C20	-2.64	1.34	1.38
2	A	600	A1AIZ	C18-C03	-2.62	1.34	1.38
2	A	600	A1AIZ	C14-C07	-2.58	1.35	1.39
2	A	600	A1AIZ	O03-C17	-2.57	1.35	1.41
2	D	600	A1AIZ	C30-C29	-2.56	1.34	1.38
2	D	600	A1AIZ	C27-C24	-2.53	1.47	1.50
2	D	600	A1AIZ	C18-C03	-2.50	1.34	1.38
2	C	600	A1AIZ	O03-C17	-2.42	1.35	1.41
2	B	600	A1AIZ	C18-C03	-2.42	1.34	1.38
2	B	600	A1AIZ	C27-C24	-2.41	1.47	1.50
2	A	600	A1AIZ	C20-C19	-2.37	1.34	1.38
2	A	600	A1AIZ	C21-C20	-2.36	1.35	1.38
2	B	600	A1AIZ	C11-C12	-2.33	1.34	1.39
2	A	600	A1AIZ	C14-C13	-2.33	1.35	1.38
2	D	600	A1AIZ	C10-C07	-2.30	1.35	1.39
2	D	600	A1AIZ	C11-C12	-2.26	1.34	1.39
2	B	600	A1AIZ	C29-C28	-2.25	1.36	1.39
2	D	600	A1AIZ	C21-C20	-2.21	1.35	1.38
2	A	600	A1AIZ	C11-C10	-2.21	1.35	1.38
2	D	600	A1AIZ	C32-C15	-2.18	1.35	1.39
2	A	600	A1AIZ	C04-C02	2.17	1.39	1.36
2	C	600	A1AIZ	C20-C19	-2.17	1.34	1.38
2	D	600	A1AIZ	C21-C17	-2.14	1.34	1.38
2	B	600	A1AIZ	C32-C15	-2.13	1.36	1.39
2	B	600	A1AIZ	C13-C12	-2.12	1.35	1.39
2	D	600	A1AIZ	C13-C12	-2.11	1.35	1.39
2	A	600	A1AIZ	C27-C24	-2.06	1.47	1.50
2	B	600	A1AIZ	C14-C13	-2.06	1.35	1.38
2	C	600	A1AIZ	C21-C20	-2.03	1.35	1.38
2	C	600	A1AIZ	O04-C22	-2.02	1.19	1.23
2	B	600	A1AIZ	C21-C17	-2.01	1.35	1.38

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	A1AIZ	C15-S01-C02	6.65	95.68	90.58
2	C	600	A1AIZ	C14-C07-C10	-6.39	110.44	118.57
2	B	600	A1AIZ	C07-C02-S01	5.52	125.81	117.69
2	D	600	A1AIZ	C15-S01-C02	5.47	94.77	90.58
2	A	600	A1AIZ	C14-C07-C10	-5.30	111.83	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	A1AIZ	C15-S01-C02	5.18	94.56	90.58
2	A	600	A1AIZ	C06-C22-N01	5.12	122.53	115.99
2	B	600	A1AIZ	C07-C02-C04	-4.97	121.84	129.93
2	C	600	A1AIZ	C06-C22-N01	4.92	122.28	115.99
2	C	600	A1AIZ	C11-C10-C07	4.64	125.75	120.80
2	C	600	A1AIZ	C13-C14-C07	4.57	125.68	120.80
2	D	600	A1AIZ	C32-C15-C28	-4.57	117.78	121.74
2	C	600	A1AIZ	C09-C06-C22	4.49	120.25	110.79
2	A	600	A1AIZ	C32-C15-C28	-4.49	117.85	121.74
2	B	600	A1AIZ	C14-C07-C10	-4.43	112.94	118.57
2	D	600	A1AIZ	C14-C07-C10	-4.39	112.98	118.57
2	D	600	A1AIZ	C07-C02-S01	4.38	124.13	117.69
2	D	600	A1AIZ	C07-C02-C04	-4.31	122.91	129.93
2	B	600	A1AIZ	C32-C15-C28	-4.23	118.07	121.74
2	A	600	A1AIZ	C13-C14-C07	4.17	125.25	120.80
2	A	600	A1AIZ	C07-C02-S01	3.98	123.55	117.69
2	C	600	A1AIZ	C07-C02-S01	3.95	123.50	117.69
2	C	600	A1AIZ	C32-C15-C28	-3.89	118.37	121.74
2	C	600	A1AIZ	C07-C02-C04	-3.87	123.63	129.93
2	C	600	A1AIZ	C15-S01-C02	3.77	93.47	90.58
2	A	600	A1AIZ	C07-C02-C04	-3.71	123.89	129.93
2	D	600	A1AIZ	C16-C24-C27	3.51	115.02	111.61
2	C	600	A1AIZ	C01-C23-N01	-3.49	102.40	112.20
2	A	600	A1AIZ	C11-C10-C07	3.38	124.41	120.80
2	C	600	A1AIZ	C30-C31-C32	-3.37	116.49	120.19
2	D	600	A1AIZ	C18-C19-C20	-3.36	115.26	120.16
2	C	600	A1AIZ	C28-C04-C02	-3.34	108.85	114.49
2	D	600	A1AIZ	C03-C18-C19	3.33	123.53	119.73
2	A	600	A1AIZ	C28-C04-C02	-3.27	108.97	114.49
2	B	600	A1AIZ	C14-C07-C02	3.25	126.01	120.84
2	C	600	A1AIZ	C31-C32-C15	3.25	123.09	118.60
2	D	600	A1AIZ	C14-C07-C02	3.21	125.95	120.84
2	B	600	A1AIZ	C01-C23-N01	-3.17	103.31	112.20
2	B	600	A1AIZ	C13-C14-C07	3.17	124.18	120.80
2	B	600	A1AIZ	C11-C10-C07	3.16	124.17	120.80
2	D	600	A1AIZ	C11-C10-C07	3.12	124.14	120.80
2	D	600	A1AIZ	C13-C14-C07	3.09	124.09	120.80
2	B	600	A1AIZ	C18-C19-C20	-3.03	115.73	120.16
2	A	600	A1AIZ	C31-C32-C15	3.00	122.75	118.60
2	B	600	A1AIZ	C25-C26-C06	2.98	116.42	111.18
2	C	600	A1AIZ	O04-C22-N01	-2.96	116.71	122.98
2	C	600	A1AIZ	C23-N01-C22	2.96	127.86	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	A1AIZ	C29-C28-C15	2.95	122.13	118.77
2	C	600	A1AIZ	C14-C07-C02	2.94	125.52	120.84
2	D	600	A1AIZ	C28-C04-C02	-2.93	109.54	114.49
2	A	600	A1AIZ	C30-C31-C32	-2.93	116.97	120.19
2	B	600	A1AIZ	C16-C24-C27	2.90	114.42	111.61
2	B	600	A1AIZ	C28-C04-C02	-2.90	109.59	114.49
2	C	600	A1AIZ	C11-C12-C13	-2.86	115.22	119.77
2	D	600	A1AIZ	C20-C21-C17	2.84	122.97	119.73
2	C	600	A1AIZ	C16-C24-C27	2.83	114.35	111.61
2	C	600	A1AIZ	C18-C19-C20	-2.82	116.04	120.16
2	D	600	A1AIZ	C29-C28-C15	2.79	121.94	118.77
2	A	600	A1AIZ	C14-C07-C02	2.79	125.27	120.84
2	A	600	A1AIZ	O04-C22-N01	-2.76	117.14	122.98
2	C	600	A1AIZ	C03-C17-C21	-2.72	116.20	120.16
2	A	600	A1AIZ	C29-C28-C15	2.68	121.82	118.77
2	A	600	A1AIZ	C11-C12-C13	-2.66	115.54	119.77
2	D	600	A1AIZ	C01-C23-N01	-2.63	104.81	112.20
2	B	600	A1AIZ	C03-C17-C21	-2.63	116.33	120.16
2	D	600	A1AIZ	C03-C17-C21	-2.62	116.34	120.16
2	C	600	A1AIZ	C21-C20-C19	2.51	122.60	119.73
2	B	600	A1AIZ	C21-C20-C19	2.34	122.41	119.73
2	B	600	A1AIZ	F02-C27-C24	2.28	115.43	112.60
2	B	600	A1AIZ	C29-C28-C04	-2.24	127.10	132.48
2	C	600	A1AIZ	C18-C03-C17	2.19	122.23	119.73
2	B	600	A1AIZ	C25-C24-C27	2.17	113.71	111.61
2	D	600	A1AIZ	C25-C26-C06	2.17	114.99	111.18
2	D	600	A1AIZ	C29-C28-C04	-2.16	127.31	132.48
2	A	600	A1AIZ	C29-C28-C04	-2.15	127.31	132.48
2	D	600	A1AIZ	O04-C22-N01	-2.14	118.45	122.98
2	C	600	A1AIZ	O05-C31-C32	2.14	125.45	119.85
2	D	600	A1AIZ	C31-C32-C15	2.14	121.56	118.60
2	D	600	A1AIZ	F01-C27-C24	-2.13	109.97	112.60
2	A	600	A1AIZ	C16-C24-C27	2.09	113.63	111.61
2	D	600	A1AIZ	C11-C12-C13	-2.06	116.49	119.77
2	A	600	A1AIZ	C25-C26-C06	2.02	114.74	111.18
2	B	600	A1AIZ	O04-C22-N01	-2.01	118.72	122.98
2	B	600	A1AIZ	C26-C25-C24	2.01	115.73	111.84

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	600	A1AIZ	C06-C22-N01-C23
2	C	600	A1AIZ	C16-C24-C27-F01
2	C	600	A1AIZ	C16-C24-C27-F02
2	C	600	A1AIZ	C16-C24-C27-F03
2	C	600	A1AIZ	C25-C24-C27-F01
2	C	600	A1AIZ	C25-C24-C27-F02
2	C	600	A1AIZ	C25-C24-C27-F03
2	C	600	A1AIZ	O04-C22-N01-C23
2	A	600	A1AIZ	C18-C19-O02-C08
2	A	600	A1AIZ	C20-C19-O02-C08
2	C	600	A1AIZ	C20-C19-O02-C08
2	C	600	A1AIZ	C18-C19-O02-C08
2	B	600	A1AIZ	C05-C01-C23-N01
2	C	600	A1AIZ	C09-C06-C22-O04
2	C	600	A1AIZ	C09-C06-C22-N01
2	D	600	A1AIZ	C05-C01-C23-N01
2	A	600	A1AIZ	C01-C23-N01-C22
2	B	600	A1AIZ	C01-C23-N01-C22
2	B	600	A1AIZ	C04-C02-C07-C10
2	D	600	A1AIZ	C04-C02-C07-C10
2	C	600	A1AIZ	C05-C08-O02-C19

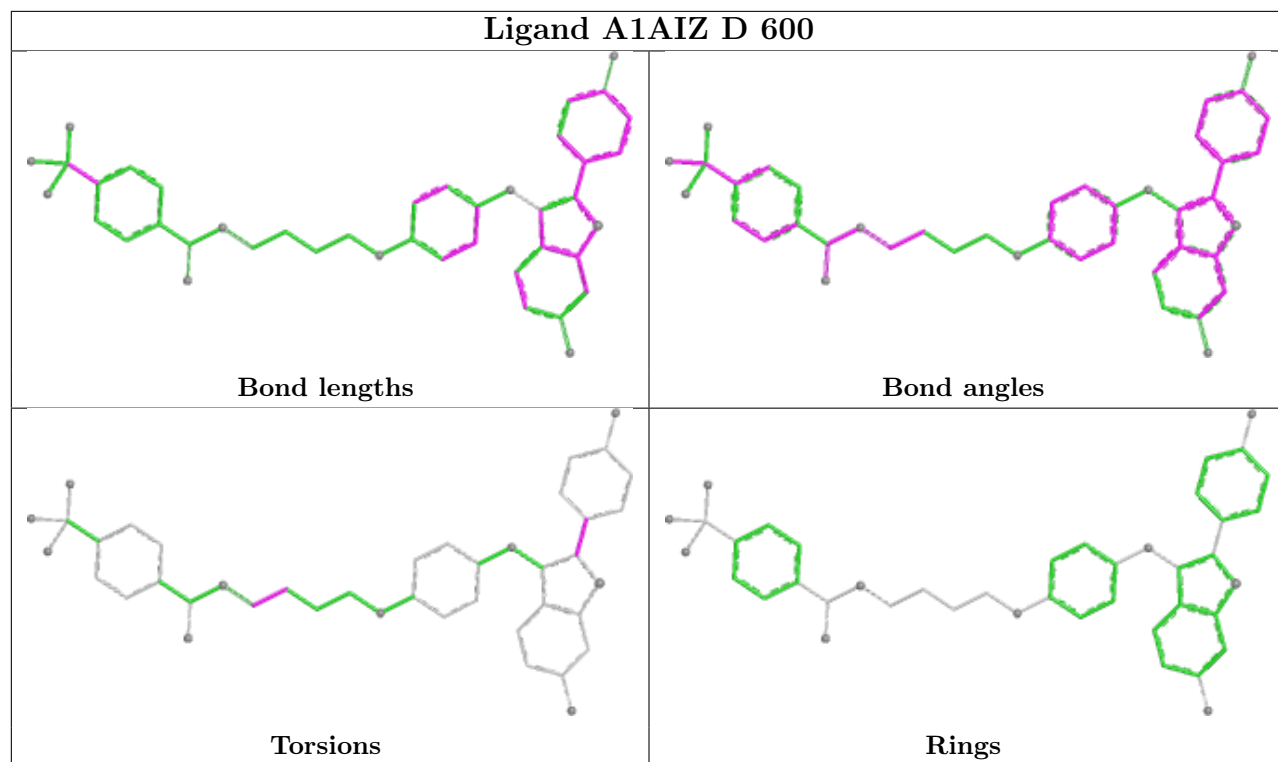
There are no ring outliers.

4 monomers are involved in 7 short contacts:

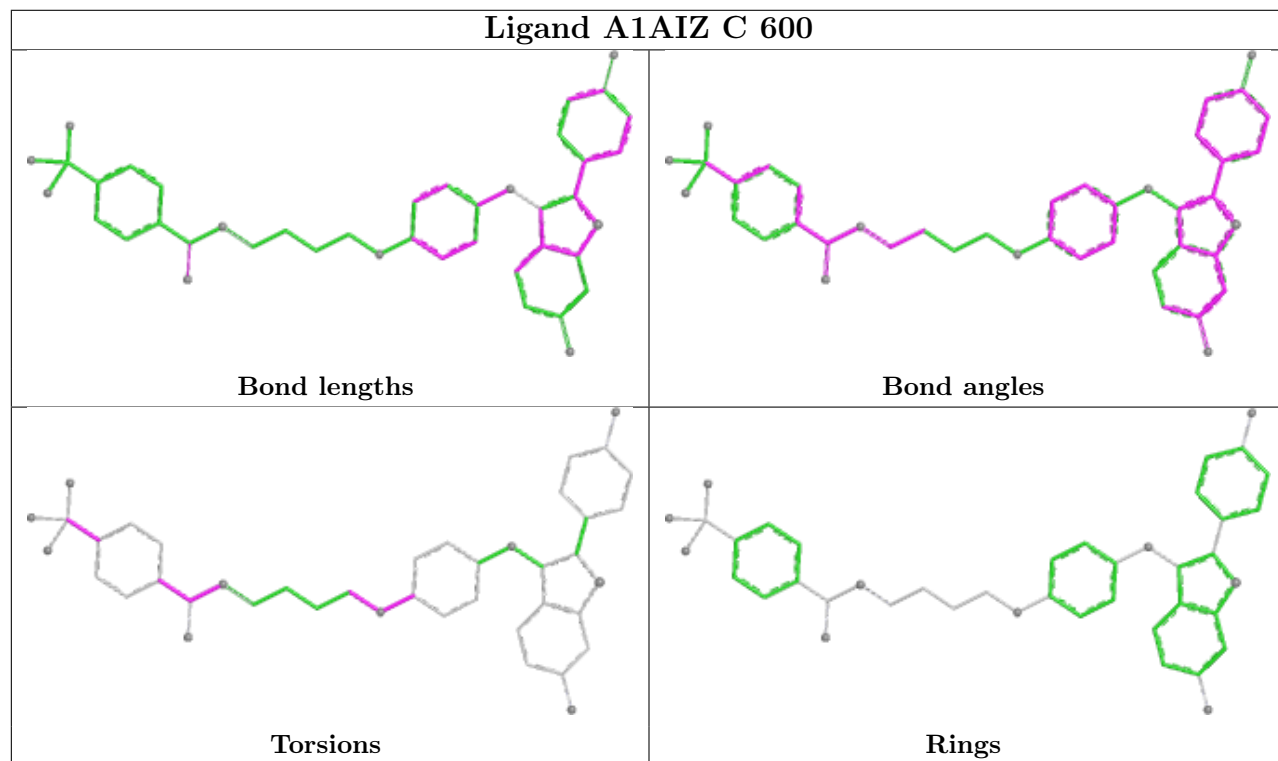
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	A1AIZ	1	0
2	C	600	A1AIZ	1	0
2	A	600	A1AIZ	4	0
2	B	600	A1AIZ	1	0

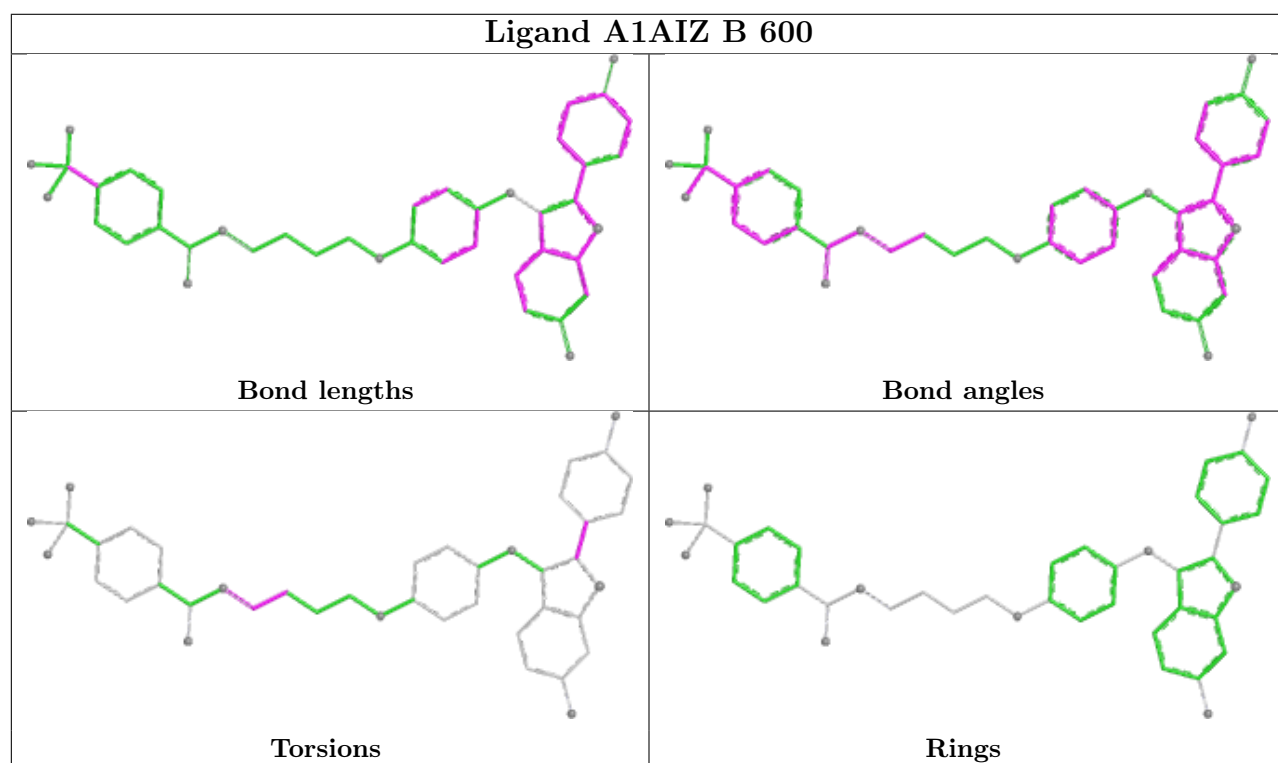
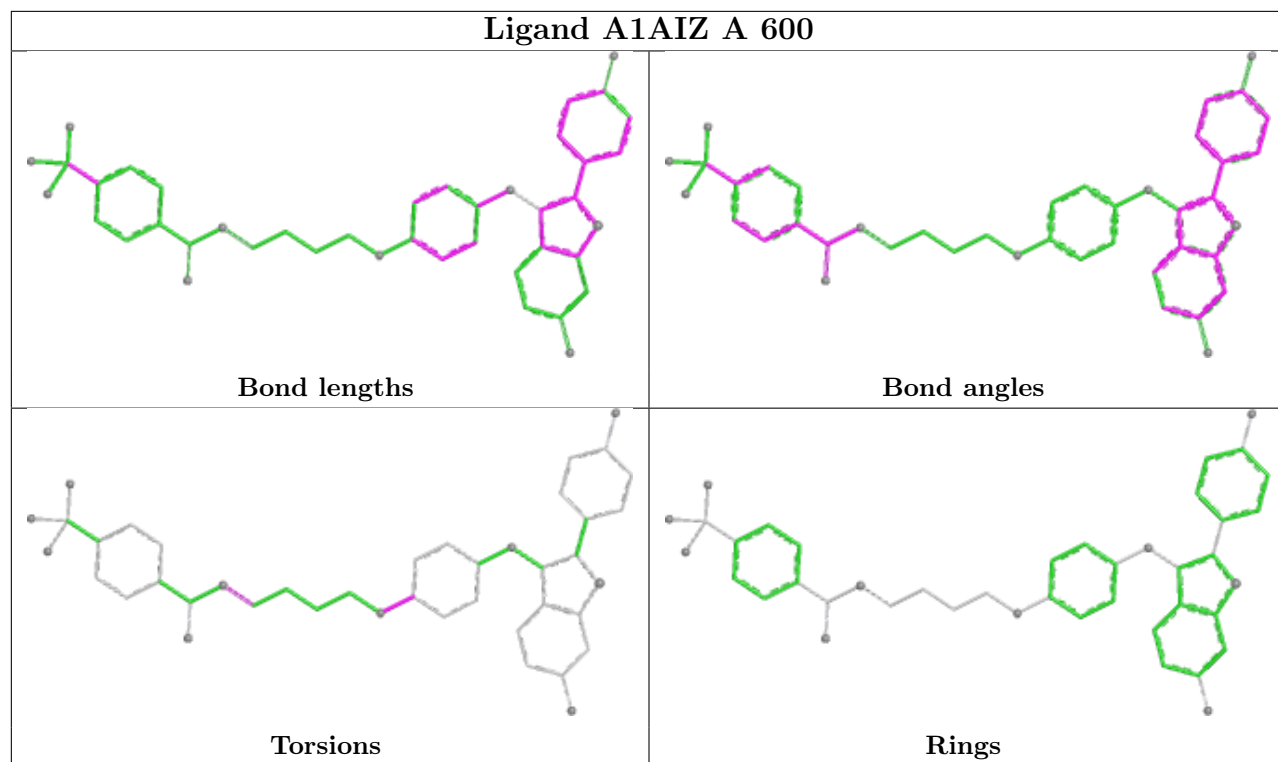
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand A1AIZ D 600



## Ligand A1AIZ C 600





## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	249/251 (99%)	-0.92	1 (0%) 88 91	11, 26, 50, 68	2 (0%)
1	B	232/251 (92%)	-0.77	1 (0%) 88 91	18, 35, 65, 87	0
1	C	249/251 (99%)	-0.90	0 100 100	11, 27, 54, 78	2 (0%)
1	D	235/251 (93%)	-0.74	2 (0%) 81 84	16, 34, 71, 89	1 (0%)
All	All	965/1004 (96%)	-0.84	4 (0%) 88 91	11, 30, 58, 89	5 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	PHE	3.8
1	B	337	PHE	3.4
1	A	462	LEU	2.3
1	D	336	PRO	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
1	YCM	B	381	10/11	0.99	0.05	21,30,68,68	0
1	YCM	D	381	10/11	0.99	0.05	18,32,82,82	0
1	YCM	C	381	10/11	1.00	0.04	12,22,61,61	0
1	YCM	A	381	10/11	1.00	0.04	12,21,57,57	0



### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

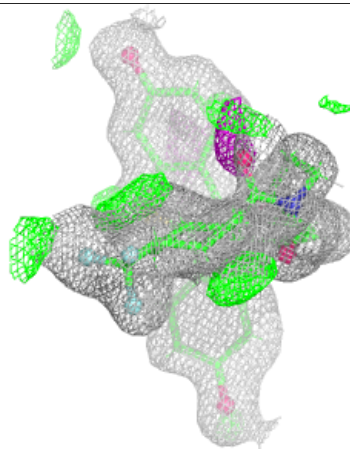
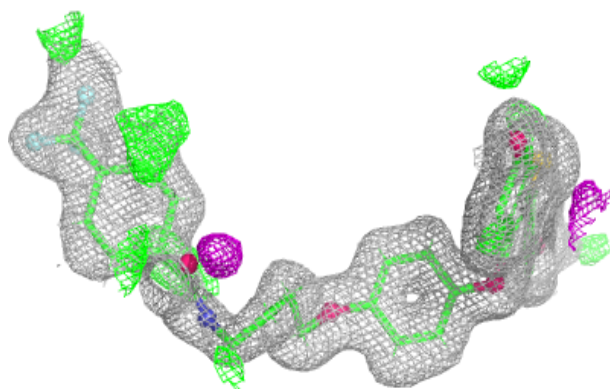
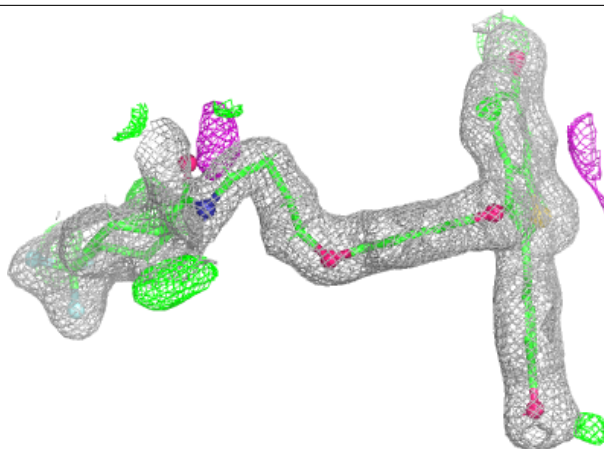
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1AIZ	A	600	42/42	0.99	0.04	11,27,49,53	0
2	A1AIZ	B	600	42/42	0.99	0.04	21,34,49,51	0
2	A1AIZ	C	600	42/42	0.99	0.04	12,28,52,59	0
2	A1AIZ	D	600	42/42	0.99	0.04	19,34,49,54	0

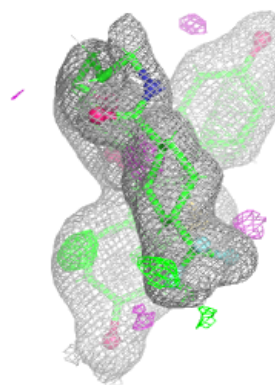
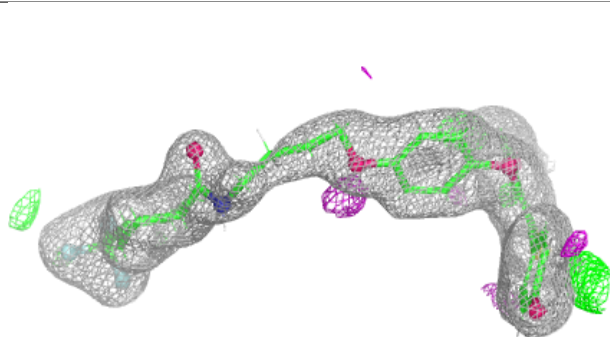
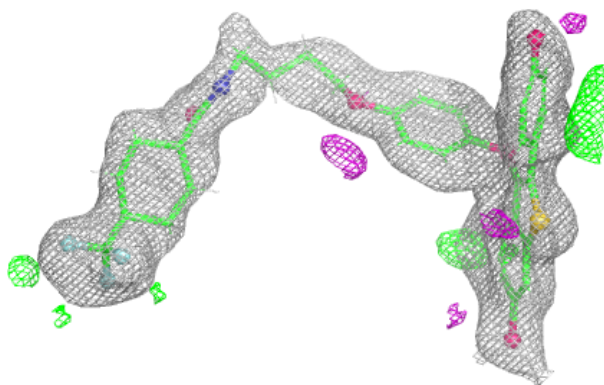
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1AIZ A 600:**

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

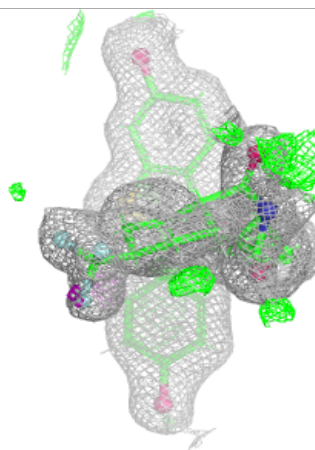
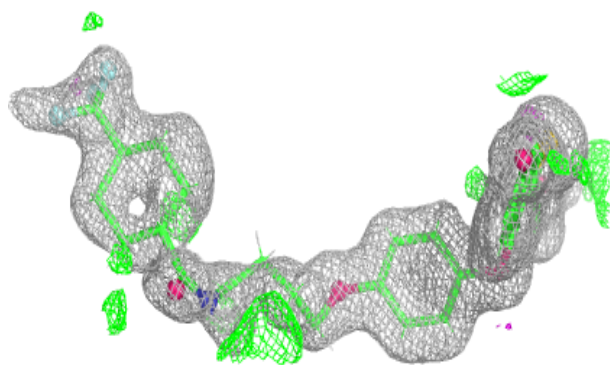
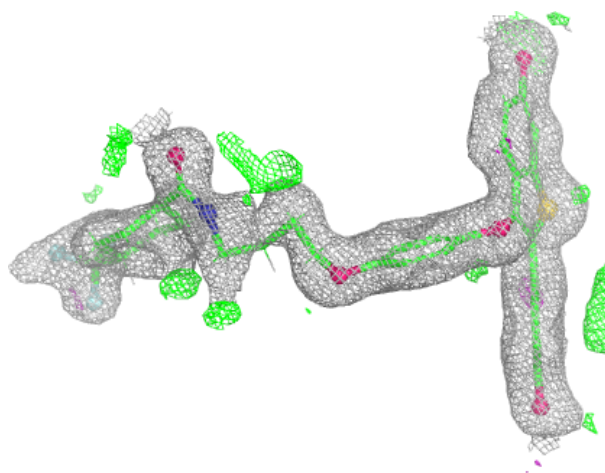
**Electron density around A1AIZ B 600:**

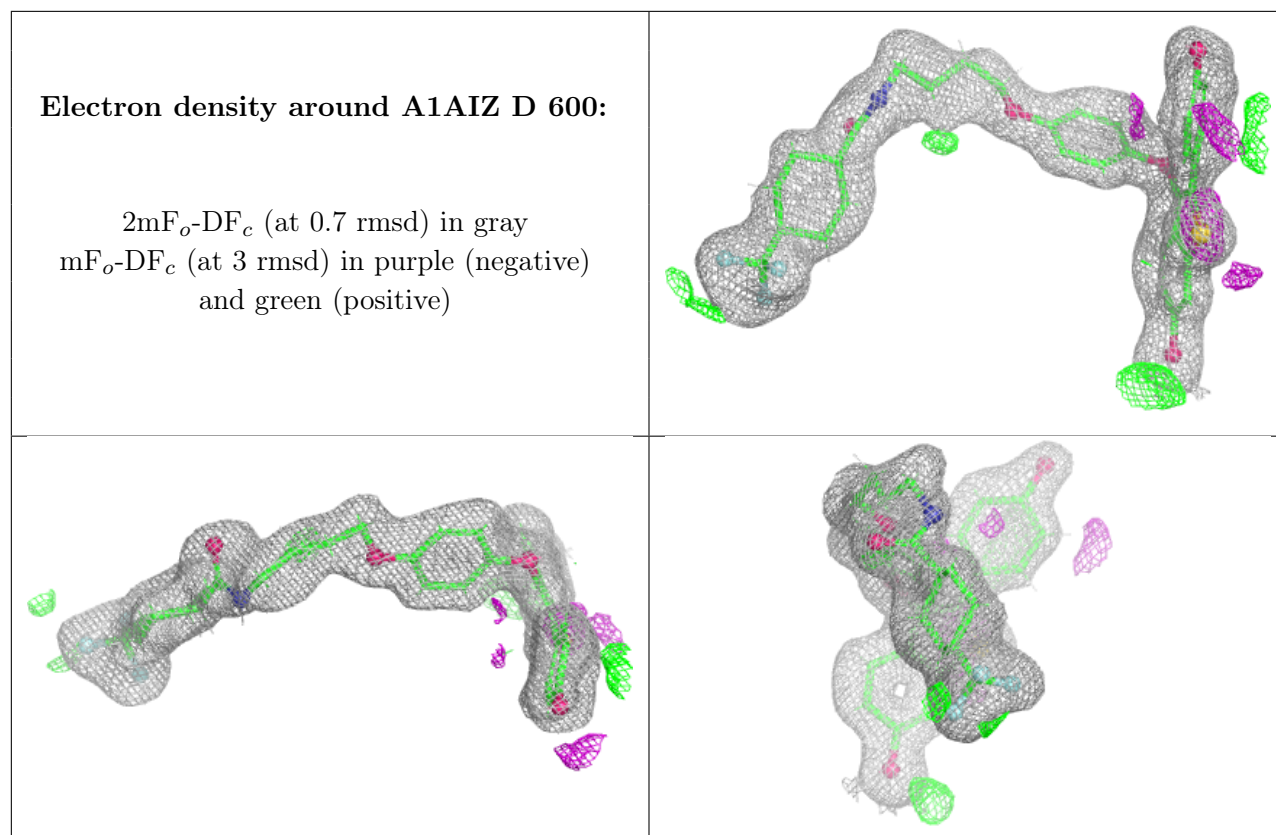
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1AIZ C 600:**

$2mF_o-DF_c$  (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.