Full wwPDB X-ray Structure Validation Report (i)

Apr 23, 2024 – 04:37 PM EDT

PDB ID	:	8V4X
Title	:	Structure of MALT1 in complex with an allosteric inhibitor
Authors	:	Judge, R.A.; Pappano, W.N.
Deposited on	:	2023-11-29
Resolution	:	2.49 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 (i) 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 (i)) were used in the production of this report:

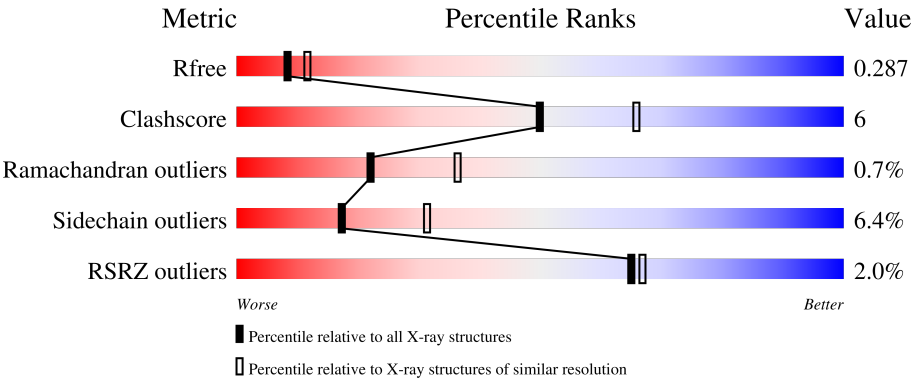
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	2% 75% 17% • 5%
1	B	387	% 77% 16% • 7%
1	C	387	3% 74% 18% • 7%
1	D	387	% 74% 20% • 5%
1	E	387	2% 80% 14% • 5%

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Mol	Chain	Length	Quality of chain
1	F	387	2% 74% 18% 7%
2	G	6	50% 33% 17%
2	H	6	50% 50%
2	I	6	83% 17%
2	J	6	67% 33%
2	K	6	100%
2	L	6	83% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17700 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 Mucosa-associated lymphoid tissue lymphoma translocation protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2853	1825	467	540	21			
1	B	360	Total	C	N	O	S	0	0	0
			2801	1790	453	538	20			
1	C	361	Total	C	N	O	S	0	0	0
			2784	1780	454	532	18			
1	D	368	Total	C	N	O	S	0	0	0
			2864	1832	469	544	19			
1	E	367	Total	C	N	O	S	0	0	0
			2814	1803	454	537	20			
1	F	358	Total	C	N	O	S	0	0	0
			2782	1779	454	529	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	SER	-	expression tag	UNP Q9UDY8
B	333	SER	-	expression tag	UNP Q9UDY8
C	333	SER	-	expression tag	UNP Q9UDY8
D	333	SER	-	expression tag	UNP Q9UDY8
E	333	SER	-	expression tag	UNP Q9UDY8
F	333	SER	-	expression tag	UNP Q9UDY8

- Molecule 2 is a protein called Inhibitor peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	0	0	1
			47	31	10	6			
2	H	6	Total	C	N	O	0	0	1
			47	31	10	6			
2	I	6	Total	C	N	O	0	0	1
			47	31	10	6			

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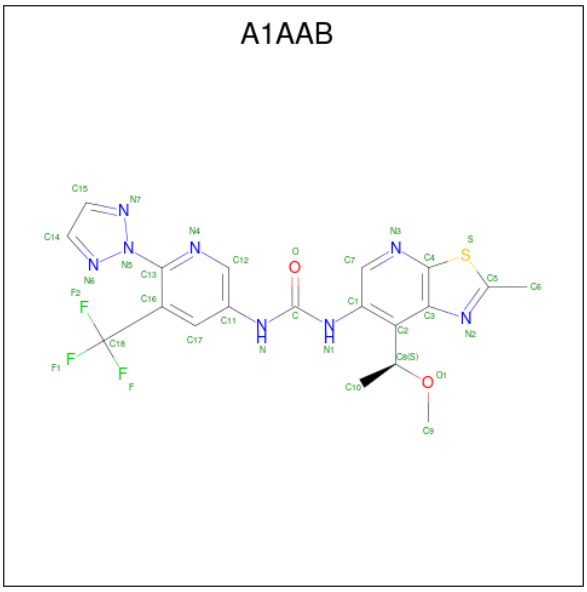
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	J	6	Total C N O 47 31 10 6	0	0	1
2	K	6	Total C N O 47 31 10 6	0	0	1
2	L	6	Total C N O 47 31 10 6	0	0	1

- Molecule 3 is N-{7-[(1S)-1-methoxyethyl]-2-methyl[1,3]thiazolo[5,4-b]pyridin-6-yl}-N'-[6-(2H-1,2,3-triazol-2-yl)-5-(trifluoromethyl)pyridin-3-yl]urea (three-letter code: A1AAB) (formula: $C_{19}H_{17}F_3N_8O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O S 33 19 3 8 2 1	0	0
3	B	1	Total C F N O S 33 19 3 8 2 1	0	0
3	C	1	Total C F N O S 33 19 3 8 2 1	0	0
3	D	1	Total C F N O S 33 19 3 8 2 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	71	Total O 71 71	0	0

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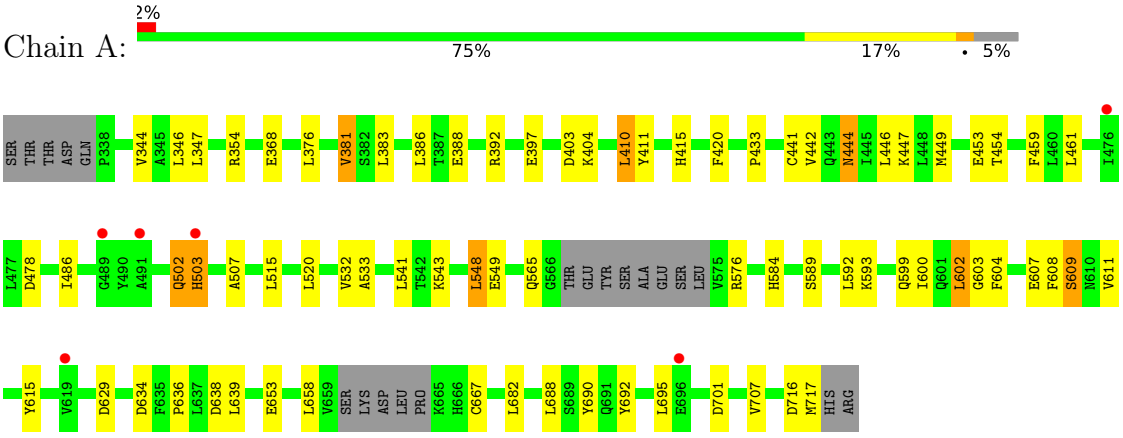
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	70	Total O 70 70	0	0
4	C	49	Total O 49 49	0	0
4	D	64	Total O 64 64	0	0
4	E	67	Total O 67 67	0	0
4	F	62	Total O 62 62	0	0
4	G	1	Total O 1 1	0	0
4	H	3	Total O 3 3	0	0
4	J	1	Total O 1 1	0	0

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.

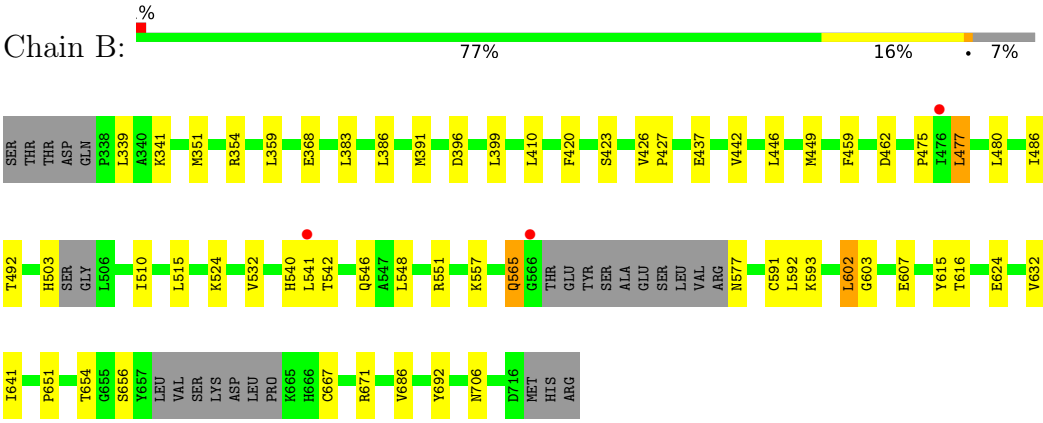
• Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1

Chain A:



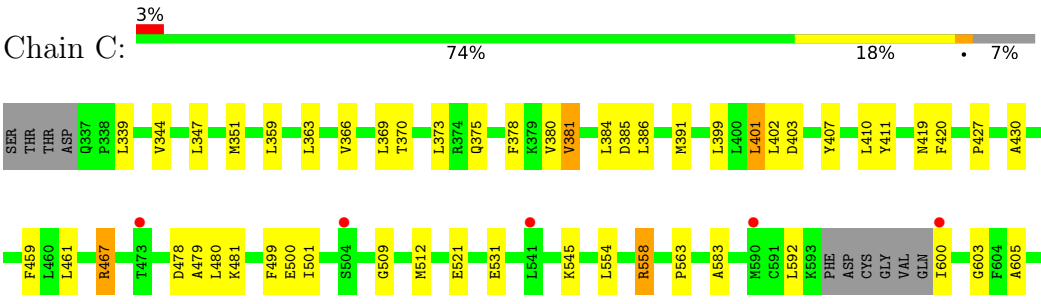
• Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1

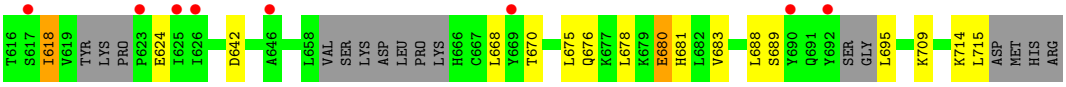
Chain B:



• Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1

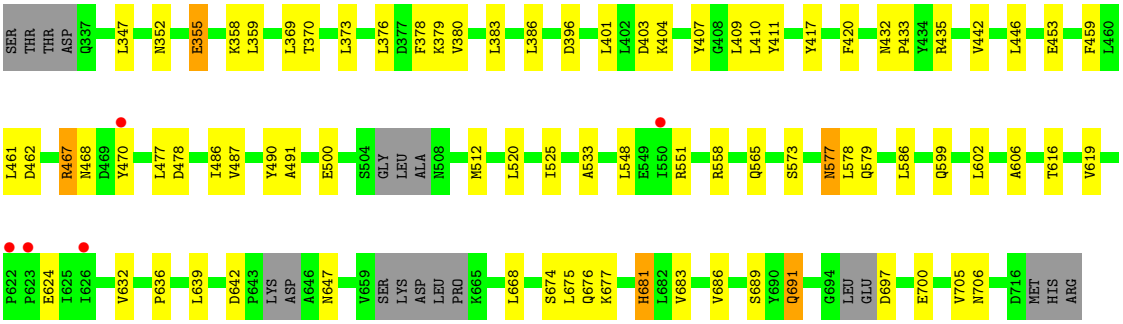
Chain C:





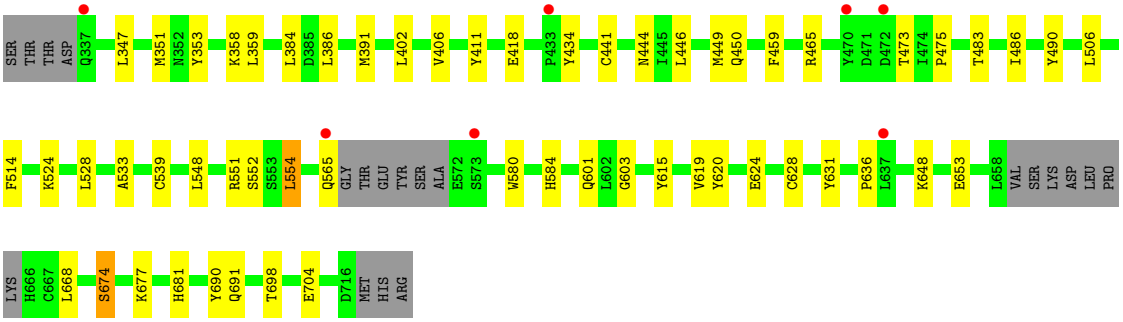
• Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1

Chain D:



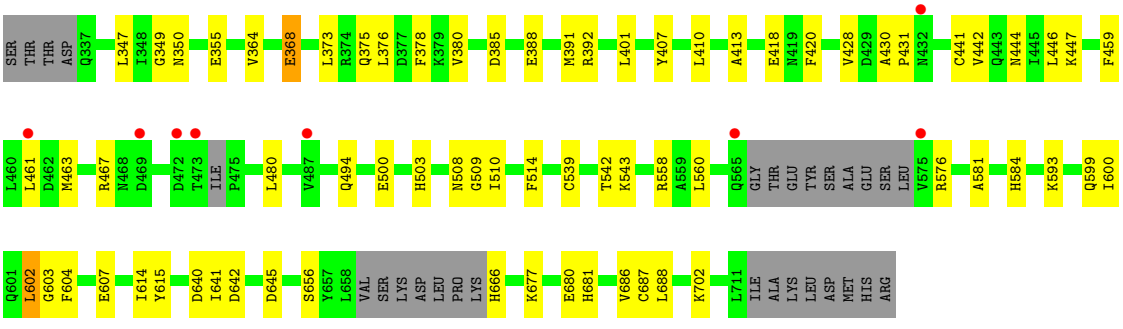
• Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1

Chain E:



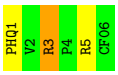
• Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1

Chain F:



• Molecule 2: Inhibitor peptide

Chain G:



• Molecule 2: Inhibitor peptide

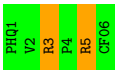
Chain H:

• Molecule 2: Inhibitor peptide

Chain I:

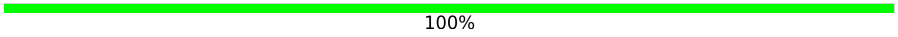
• Molecule 2: Inhibitor peptide

Chain J:



• Molecule 2: Inhibitor peptide

Chain K:



There are no outlier residues recorded for this chain.

• Molecule 2: Inhibitor peptide

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.32Å 78.77Å 135.88Å 90.00° 112.52° 90.00°	Depositor
Resolution (Å)	34.90 – 2.49 34.90 – 2.49	Depositor EDS
% Data completeness (in resolution range)	54.7 (34.90-2.49) 54.7 (34.90-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.209 , 0.285 0.209 , 0.287	Depositor DCC
R_{free} test set	2471 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17700	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4447e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AAB, PHQ, CF0

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	0.36	0/2905	0.56	0/3936
1	B	0.36	0/2852	0.56	0/3868
1	C	0.34	0/2831	0.55	0/3835
1	D	0.36	0/2915	0.57	0/3949
1	E	0.36	0/2866	0.58	0/3890
1	F	0.36	0/2833	0.56	0/3839
2	G	0.35	0/36	0.71	0/47
2	H	0.34	0/36	0.74	0/47
2	I	0.35	0/36	0.62	0/47
2	J	0.31	0/36	0.60	0/47
2	K	0.33	0/36	0.61	0/47
2	L	0.28	0/36	0.62	0/47
All	All	0.36	0/17418	0.56	0/23599

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
2	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	3	ARG	Sidechain

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	2853	0	2804	36	0
1	B	2801	0	2721	30	0
1	C	2784	0	2718	41	0
1	D	2864	0	2805	40	0
1	E	2814	0	2722	25	0
1	F	2782	0	2712	33	0
2	G	47	0	48	4	0
2	H	47	0	48	1	0
2	I	47	0	48	1	0
2	J	47	0	48	2	0
2	K	47	0	48	0	0
2	L	47	0	48	1	0
3	A	33	0	0	0	0
3	B	33	0	0	0	0
3	C	33	0	0	4	0
3	D	33	0	0	1	0
4	A	71	0	0	1	0
4	B	70	0	0	0	0
4	C	49	0	0	0	0
4	D	64	0	0	0	0
4	E	67	0	0	0	0
4	F	62	0	0	1	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
4	J	1	0	0	0	0
All	All	17700	0	16770	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (198) 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:447:LYS:NZ	1:A:478:ASP:HB2	1.87	0.88
1:A:447:LYS:HZ1	1:A:478:ASP:HB2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:581:ALA:HA	1:F:584:HIS:NE2	1.97	0.79
1:A:502:GLN:HA	2:G:3:ARG:HG2	1.67	0.75
1:C:680:GLU:HA	1:C:709:LYS:HE2	1.66	0.75
1:D:681:HIS:CD2	1:D:706:ASN:HD21	2.05	0.74
1:D:355:GLU:HG2	1:D:432:ASN:HB3	1.72	0.70
1:F:593:LYS:HG3	1:F:599:GLN:HG2	1.75	0.68
1:D:407:TYR:OH	1:D:558:ARG:NH1	2.26	0.67
1:B:551:ARG:HG2	1:D:551:ARG:HG2	1.77	0.65
1:C:381:VAL:HG11	3:C:901:A1AAB:C3	2.28	0.64
1:C:347:LEU:HG	1:C:411:TYR:HB3	1.80	0.64
1:A:608:PHE:HB2	1:A:611:VAL:HB	1.79	0.62
1:A:447:LYS:HZ3	1:A:478:ASP:HB2	1.64	0.62
1:B:632:VAL:HG12	1:B:686:VAL:HG22	1.81	0.62
1:C:500:GLU:HA	1:C:509:GLY:HA2	1.82	0.62
1:E:580:TRP:HE1	1:E:584:HIS:HE1	1.48	0.62
1:C:407:TYR:OH	1:C:558:ARG:NH1	2.32	0.61
1:A:507:ALA:HB2	1:B:540:HIS:CE1	2.36	0.61
1:D:352:ASN:HA	1:D:358:LYS:HD3	1.81	0.61
1:E:648:LYS:HE3	1:E:653:GLU:HB3	1.83	0.61
1:B:510:ILE:HG13	1:B:542:THR:HG21	1.83	0.60
1:D:369:LEU:HD13	1:D:512:MET:HE1	1.83	0.60
1:C:339:LEU:HD23	1:C:563:PRO:HG2	1.83	0.60
1:C:381:VAL:CG1	3:C:901:A1AAB:C4	2.80	0.59
1:F:446:LEU:HD12	1:F:480:LEU:HD13	1.84	0.59
1:C:373:LEU:O	1:C:378:PHE:HB2	2.02	0.59
1:D:442:VAL:HG11	1:D:461:LEU:HD11	1.85	0.59
1:F:364:VAL:O	1:F:368:GLU:HG2	2.03	0.57
1:D:632:VAL:HG12	1:D:686:VAL:HG22	1.86	0.57
1:A:420:PHE:HB3	1:C:420:PHE:HB3	1.86	0.57
1:B:524:LYS:HD2	1:B:557:LYS:HA	1.86	0.57
1:C:427:PRO:HD2	1:C:430:ALA:HB2	1.86	0.57
1:B:423:SER:HB2	1:B:442:VAL:HB	1.86	0.56
1:F:510:ILE:HG13	1:F:542:THR:HG21	1.85	0.56
1:E:674:SER:HB2	1:E:677:LYS:HD3	1.88	0.56
1:A:442:VAL:HG11	1:A:461:LEU:HD11	1.89	0.55
1:C:676:GLN:HB2	3:C:901:A1AAB:N6	2.21	0.55
1:C:347:LEU:HD21	1:C:369:LEU:HB3	1.88	0.55
1:C:381:VAL:HG11	3:C:901:A1AAB:C4	2.37	0.54
1:F:602:LEU:HD11	1:F:686:VAL:HG21	1.89	0.54
1:C:605:ALA:HB3	1:C:613:ILE:HG23	1.90	0.54
1:F:642:ASP:HB3	1:F:645:ASP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:602:LEU:HD21	1:D:616:THR:HG22	1.89	0.54
1:A:446:LEU:HD11	1:A:486:ILE:HG12	1.89	0.54
1:D:373:LEU:HD21	1:D:409:LEU:HD22	1.89	0.53
1:D:359:LEU:HD13	2:J:5:ARG:HG3	1.91	0.53
1:F:441:CYS:HB3	1:F:444:ASN:HD22	1.74	0.53
1:C:351:MET:HB3	1:C:359:LEU:O	2.09	0.53
1:C:600:ILE:HD11	1:C:688:LEU:HD13	1.89	0.53
1:F:600:ILE:HD11	1:F:688:LEU:HD13	1.90	0.53
1:A:592:LEU:HD13	1:A:602:LEU:HD13	1.91	0.52
1:E:580:TRP:NE1	1:E:584:HIS:HE1	2.06	0.52
1:B:341:LYS:HA	1:B:565:GLN:HG2	1.91	0.52
1:B:386:LEU:HB2	1:B:391:MET:HG3	1.92	0.52
1:E:490:TYR:HE1	1:E:551:ARG:HD2	1.75	0.52
1:D:500:GLU:HG3	2:J:3:ARG:HG3	1.92	0.51
1:F:373:LEU:O	1:F:378:PHE:HB2	2.10	0.51
1:C:521:GLU:OE1	1:C:531:GLU:OE1	2.28	0.51
1:B:420:PHE:HB3	1:D:420:PHE:HB3	1.92	0.51
1:D:674:SER:HB2	1:D:677:LYS:NZ	2.25	0.51
1:E:465:ARG:HH22	1:E:551:ARG:NH2	2.09	0.51
1:B:383:LEU:HB3	1:B:386:LEU:HD21	1.92	0.51
1:B:475:PRO:HB2	1:B:477:LEU:HD12	1.92	0.51
1:D:462:ASP:HA	1:D:491:ALA:HB2	1.92	0.51
1:C:386:LEU:HB2	1:C:391:MET:HG3	1.93	0.51
1:C:442:VAL:HG11	1:C:461:LEU:HD11	1.92	0.51
1:A:397:GLU:OE2	1:F:503:HIS:HE1	1.95	0.50
1:E:580:TRP:NE1	1:E:584:HIS:CE1	2.78	0.50
1:C:347:LEU:HD21	1:C:369:LEU:HD23	1.93	0.50
1:A:449:MET:SD	1:A:459:PHE:CZ	3.05	0.50
1:B:656:SER:HB3	1:B:671:ARG:HD2	1.93	0.50
1:F:349:GLY:HA2	1:F:413:ALA:O	2.11	0.49
1:A:593:LYS:HG3	1:A:599:GLN:HG2	1.93	0.49
1:F:446:LEU:HD23	1:F:459:PHE:HE1	1.76	0.49
1:C:420:PHE:CE1	1:C:467:ARG:NH1	2.78	0.49
1:D:676:GLN:HB2	3:D:901:A1AAB:N6	2.28	0.49
1:B:396:ASP:HA	1:B:399:LEU:HD12	1.95	0.49
1:A:347:LEU:HG	1:A:411:TYR:HB3	1.95	0.49
1:A:690:TYR:HE1	1:A:701:ASP:HB2	1.78	0.48
1:B:492:THR:HB	1:B:546:GLN:HG3	1.96	0.48
1:B:541:LEU:HD12	2:G:1:PHQ:H81	1.95	0.48
1:C:612:MET:HB2	1:C:675:LEU:HD11	1.95	0.48
1:B:341:LYS:HA	1:B:565:GLN:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:GLU:HG3	1:F:508:ASN:HD21	1.78	0.48
1:D:373:LEU:O	1:D:378:PHE:HB2	2.14	0.48
1:A:515:LEU:HD12	1:A:532:VAL:HG21	1.95	0.48
1:F:376:LEU:HD13	1:F:560:LEU:HB3	1.96	0.48
1:B:449:MET:SD	1:B:459:PHE:CZ	3.06	0.47
1:A:507:ALA:HB2	1:B:540:HIS:ND1	2.28	0.47
1:D:379:LYS:NZ	1:D:577:ASN:HB2	2.29	0.47
1:F:347:LEU:HD13	1:F:380:VAL:HG13	1.95	0.47
1:D:347:LEU:HD21	1:D:369:LEU:HD23	1.95	0.47
1:A:603:GLY:HA3	1:A:615:TYR:CE1	2.49	0.47
1:E:473:THR:O	1:E:475:PRO:HD3	2.12	0.47
1:F:607:GLU:OE1	1:F:656:SER:HB2	2.15	0.47
1:F:388:GLU:O	1:F:392:ARG:HG3	2.15	0.47
1:F:442:VAL:HG11	1:F:461:LEU:HD11	1.97	0.47
1:C:614:ILE:HG13	1:C:670:THR:HB	1.97	0.47
1:A:376:LEU:HG	1:A:520:LEU:HD23	1.97	0.46
1:C:344:VAL:HG11	1:C:401:LEU:HD12	1.95	0.46
1:D:404:LYS:HG2	1:D:453:GLU:HB3	1.96	0.46
1:D:636:PRO:HD2	1:D:639:LEU:HD12	1.96	0.46
1:E:603:GLY:HA3	1:E:615:TYR:CE2	2.50	0.46
1:D:446:LEU:HD13	1:D:459:PHE:HE2	1.80	0.46
1:C:446:LEU:HD13	1:C:459:PHE:HE2	1.80	0.46
1:A:636:PRO:HD2	1:A:639:LEU:HD12	1.97	0.46
1:B:480:LEU:HD22	1:B:480:LEU:H	1.79	0.46
1:D:417:TYR:CD2	1:D:468:ASN:HB2	2.51	0.46
1:C:501:ILE:HG23	2:I:1:PHQ:H81	1.98	0.46
1:D:435:ARG:NE	1:D:470:TYR:HE2	2.14	0.46
1:F:364:VAL:O	1:F:368:GLU:CG	2.64	0.46
1:D:691:GLN:HE21	1:D:697:ASP:N	2.14	0.45
1:A:600:ILE:HD11	1:A:688:LEU:HD13	1.97	0.45
1:F:373:LEU:HD23	1:F:376:LEU:HD12	1.98	0.45
1:C:369:LEU:HD13	1:C:512:MET:HE1	1.99	0.45
1:C:499:PHE:HE2	1:C:545:LYS:HB2	1.82	0.45
1:A:383:LEU:HB3	1:A:386:LEU:HD21	1.98	0.45
1:A:441:CYS:HB3	1:A:444:ASN:HB2	1.99	0.45
1:C:583:ALA:HB2	1:C:715:LEU:HD13	1.98	0.45
1:E:450:GLN:NE2	1:E:483:THR:OG1	2.50	0.45
1:E:691:GLN:HG2	1:E:698:THR:HA	1.97	0.45
1:E:347:LEU:HG	1:E:411:TYR:HB3	1.99	0.45
1:E:446:LEU:HD21	1:E:486:ILE:HD13	1.99	0.45
1:E:351:MET:HB3	1:E:359:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:GLU:HG3	1:B:692:TYR:HD2	1.82	0.44
1:B:651:PRO:O	1:B:654:THR:OG1	2.29	0.44
1:F:687:CYS:HB3	1:F:702:LYS:HG2	1.99	0.44
1:A:533:ALA:HB2	1:A:548:LEU:HD23	1.98	0.44
1:F:500:GLU:OE1	2:L:5:ARG:NH2	2.50	0.44
1:B:603:GLY:HA3	1:B:615:TYR:CZ	2.53	0.44
1:C:419:ASN:OD1	1:C:467:ARG:HG2	2.18	0.44
1:D:373:LEU:HB3	1:D:380:VAL:HG21	2.00	0.44
1:E:441:CYS:HB3	1:E:444:ASN:OD1	2.18	0.44
1:B:462:ASP:HA	1:B:491:ALA:HB2	2.00	0.43
1:F:350:ASN:HB3	1:F:428:VAL:HG23	1.99	0.43
1:A:344:VAL:HG11	1:A:576:ARG:HD3	1.99	0.43
1:C:380:VAL:HG12	1:C:381:VAL:N	2.34	0.43
1:D:533:ALA:HB2	1:D:548:LEU:HD23	1.99	0.43
1:D:647:ASN:HB3	1:D:668:LEU:HD13	1.99	0.43
1:E:446:LEU:HD13	1:E:459:PHE:HE1	1.83	0.43
1:F:407:TYR:OH	1:F:558:ARG:NH1	2.45	0.43
1:E:514:PHE:CZ	1:E:539:CYS:HB2	2.53	0.43
1:F:420:PHE:HB2	4:F:824:HOH:O	2.18	0.43
1:A:388:GLU:O	1:A:392:ARG:HG3	2.19	0.43
1:A:381:VAL:HG23	1:A:584:HIS:HE1	1.84	0.43
1:A:404:LYS:HA	1:A:453:GLU:O	2.19	0.43
1:B:515:LEU:HD12	1:B:532:VAL:HG21	2.01	0.43
1:B:603:GLY:HA3	1:B:615:TYR:CE1	2.53	0.43
1:B:592:LEU:HD12	1:B:602:LEU:HD13	2.01	0.43
1:C:366:VAL:O	1:C:370:THR:OG1	2.28	0.42
1:C:363:LEU:HG	1:C:384:LEU:HD11	2.01	0.42
1:E:449:MET:SD	1:E:459:PHE:CZ	3.12	0.42
1:F:500:GLU:HA	1:F:509:GLY:HA2	2.01	0.42
1:D:487:VAL:HG21	1:D:525:ILE:HG23	2.02	0.42
1:E:402:LEU:HA	1:E:406:VAL:HG11	2.01	0.42
1:A:602:LEU:HD23	1:A:604:PHE:CZ	2.54	0.42
1:D:383:LEU:HB3	1:D:386:LEU:HD21	2.01	0.42
1:F:604:PHE:HD1	1:F:614:ILE:HG12	1.85	0.42
1:A:415:HIS:HA	2:G:5:ARG:O	2.20	0.42
1:B:351:MET:HB3	1:B:359:LEU:O	2.19	0.42
1:B:503:HIS:HB2	2:H:1:PHQ:H61	2.00	0.42
1:A:503:HIS:HB3	2:G:3:ARG:HH11	1.85	0.42
1:A:682:LEU:HB3	1:A:707:VAL:HG22	2.01	0.42
1:B:446:LEU:HD11	1:B:486:ILE:HG12	2.01	0.42
1:C:399:LEU:HD23	1:C:402:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:LYS:HG2	1:D:453:GLU:CB	2.49	0.42
1:C:554:LEU:HD11	1:C:558:ARG:HG3	2.01	0.42
1:D:347:LEU:HG	1:D:411:TYR:HB3	2.01	0.41
1:D:573:SER:O	1:D:577:ASN:HB3	2.20	0.41
1:E:524:LYS:HE3	1:E:554:LEU:HD23	2.01	0.41
1:F:603:GLY:HA3	1:F:615:TYR:CE1	2.55	0.41
1:E:353:TYR:O	1:E:358:LYS:HE2	2.21	0.41
1:F:368:GLU:OE1	1:F:508:ASN:OD1	2.39	0.41
1:A:433:PRO:HD3	1:E:620:TYR:CG	2.55	0.41
1:C:592:LEU:HB2	1:C:600:ILE:HB	2.01	0.41
1:C:592:LEU:HD23	1:C:600:ILE:HG22	2.02	0.41
1:C:618:ILE:H	1:C:618:ILE:HG13	1.66	0.41
1:D:490:TYR:O	1:D:548:LEU:HD12	2.21	0.41
1:E:386:LEU:HB2	1:E:391:MET:HG3	2.02	0.41
1:E:533:ALA:HB2	1:E:548:LEU:HD23	2.03	0.41
1:C:347:LEU:HB3	1:C:366:VAL:HG13	2.02	0.41
1:D:446:LEU:HD11	1:D:486:ILE:HG12	2.01	0.41
1:D:586:LEU:HD11	1:D:606:ALA:H	1.85	0.41
1:D:674:SER:HB2	1:D:677:LYS:HZ2	1.86	0.41
1:F:401:LEU:O	1:F:576:ARG:HD3	2.21	0.41
1:D:420:PHE:CE1	1:D:467:ARG:NH1	2.89	0.41
1:E:628:CYS:HB3	1:E:690:TYR:HA	2.02	0.41
1:D:432:ASN:HA	1:D:433:PRO:HA	1.96	0.40
1:A:346:LEU:HD23	1:A:410:LEU:HD12	2.04	0.40
1:A:692:TYR:HB2	1:A:695:LEU:HB2	2.02	0.40
1:B:426:VAL:HA	1:B:427:PRO:HD3	1.98	0.40
1:A:584:HIS:NE2	1:A:609:SER:OG	2.54	0.40
4:A:1016:HOH:O	1:C:480:LEU:HB2	2.21	0.40
1:F:430:ALA:HA	1:F:431:PRO:HD3	1.93	0.40
1:C:603:GLY:HA3	1:C:615:TYR:CE2	2.56	0.40
1:F:514:PHE:CZ	1:F:539:CYS:HB2	2.56	0.40
1:D:376:LEU:HD21	1:D:520:LEU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/387 (93%)	337 (93%)	20 (6%)	4 (1%)	14	23
1	B	352/387 (91%)	326 (93%)	26 (7%)	0	100	100
1	C	351/387 (91%)	327 (93%)	20 (6%)	4 (1%)	14	23
1	D	358/387 (92%)	332 (93%)	26 (7%)	0	100	100
1	E	361/387 (93%)	337 (93%)	20 (6%)	4 (1%)	14	23
1	F	350/387 (90%)	328 (94%)	18 (5%)	4 (1%)	14	23
2	G	2/6 (33%)	2 (100%)	0	0	100	100
2	H	2/6 (33%)	2 (100%)	0	0	100	100
2	I	2/6 (33%)	2 (100%)	0	0	100	100
2	J	2/6 (33%)	2 (100%)	0	0	100	100
2	K	2/6 (33%)	2 (100%)	0	0	100	100
2	L	2/6 (33%)	2 (100%)	0	0	100	100
All	All	2145/2358 (91%)	1999 (93%)	130 (6%)	16 (1%)	22	36

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	681	HIS
1	E	434	TYR
1	E	674	SER
1	F	681	HIS
1	A	503	HIS
1	A	716	ASP
1	E	554	LEU
1	A	502	GLN
1	C	479	ALA
1	F	680	GLU
1	C	385	ASP
1	F	385	ASP
1	F	640	ASP
1	C	680	GLU
1	A	634	ASP
1	E	636	PRO

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	308/344 (90%)	286 (93%)	22 (7%)	14 26
1	B	302/344 (88%)	283 (94%)	19 (6%)	18 32
1	C	297/344 (86%)	276 (93%)	21 (7%)	14 26
1	D	309/344 (90%)	285 (92%)	24 (8%)	12 22
1	E	298/344 (87%)	285 (96%)	13 (4%)	28 49
1	F	299/344 (87%)	284 (95%)	15 (5%)	24 43
2	G	4/4 (100%)	3 (75%)	1 (25%)	0 1
2	H	4/4 (100%)	3 (75%)	1 (25%)	0 1
2	I	4/4 (100%)	4 (100%)	0	100 100
2	J	4/4 (100%)	2 (50%)	2 (50%)	0 0
2	K	4/4 (100%)	4 (100%)	0	100 100
2	L	4/4 (100%)	4 (100%)	0	100 100
All	All	1837/2088 (88%)	1719 (94%)	118 (6%)	17 31

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ARG
1	A	368	GLU
1	A	381	VAL
1	A	403	ASP
1	A	410	LEU
1	A	444	ASN
1	A	454	THR
1	A	541	LEU
1	A	543	LYS
1	A	548	LEU
1	A	549	GLU
1	A	565	GLN
1	A	589	SER
1	A	602	LEU

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Mol	Chain	Res	Type
1	A	607	GLU
1	A	609	SER
1	A	629	ASP
1	A	638	ASP
1	A	653	GLU
1	A	658	LEU
1	A	667	CYS
1	A	717	MET
1	B	339	LEU
1	B	354	ARG
1	B	368	GLU
1	B	410	LEU
1	B	437	GLU
1	B	477	LEU
1	B	548	LEU
1	B	565	GLN
1	B	577	ASN
1	B	591	CYS
1	B	593	LYS
1	B	602	LEU
1	B	607	GLU
1	B	616	THR
1	B	633	THR
1	B	638	ASP
1	B	641	ILE
1	B	667	CYS
1	B	706	ASN
1	C	375	GLN
1	C	381	VAL
1	C	401	LEU
1	C	403	ASP
1	C	410	LEU
1	C	447	LYS
1	C	467	ARG
1	C	478	ASP
1	C	481	LYS
1	C	558	ARG
1	C	612	MET
1	C	613	ILE
1	C	618	ILE
1	C	624	GLU
1	C	642	ASP

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Mol	Chain	Res	Type
1	C	668	LEU
1	C	678	LEU
1	C	683	VAL
1	C	689	SER
1	C	695	LEU
1	C	714	LYS
1	D	355	GLU
1	D	370	THR
1	D	396	ASP
1	D	401	LEU
1	D	403	ASP
1	D	410	LEU
1	D	467	ARG
1	D	477	LEU
1	D	478	ASP
1	D	565	GLN
1	D	577	ASN
1	D	578	LEU
1	D	579	GLN
1	D	599	GLN
1	D	619	VAL
1	D	624	GLU
1	D	642	ASP
1	D	675	LEU
1	D	681	HIS
1	D	683	VAL
1	D	689	SER
1	D	691	GLN
1	D	700	GLU
1	D	705	VAL
1	E	384	LEU
1	E	418	GLU
1	E	506	LEU
1	E	528	LEU
1	E	552	SER
1	E	565	GLN
1	E	601	GLN
1	E	619	VAL
1	E	624	GLU
1	E	631	TYR
1	E	668	LEU
1	E	681	HIS

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Mol	Chain	Res	Type
1	E	704	GLU
1	F	355	GLU
1	F	368	GLU
1	F	375	GLN
1	F	391	MET
1	F	410	LEU
1	F	418	GLU
1	F	447	LYS
1	F	463	MET
1	F	467	ARG
1	F	494	GLN
1	F	543	LYS
1	F	602	LEU
1	F	641	ILE
1	F	666	HIS
1	F	677	LYS
2	G	3	ARG
2	H	2	VAL
2	J	3	ARG
2	J	5	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	ASN
1	A	444	ASN
1	B	494	GLN
1	B	666	HIS
1	B	706	ASN
1	C	502	GLN
1	C	584	HIS
1	D	371	ASN
1	D	508	ASN
1	D	681	HIS
1	E	371	ASN
1	E	503	HIS
1	E	584	HIS
1	F	375	GLN
1	F	444	ASN
1	F	565	GLN
1	F	599	GLN
1	F	703	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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	A1AAB	D	901	-	30,36,36	0.92	1 (3%)	30,53,53	0.70	1 (3%)
3	A1AAB	C	901	-	30,36,36	0.96	1 (3%)	30,53,53	0.81	1 (3%)
3	A1AAB	A	901	-	30,36,36	0.87	1 (3%)	30,53,53	0.73	1 (3%)
3	A1AAB	B	901	-	30,36,36	1.10	2 (6%)	30,53,53	0.63	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
3	A1AAB	D	901	-	-	5/20/24/24	0/4/4/4
3	A1AAB	C	901	-	-	6/20/24/24	0/4/4/4
3	A1AAB	A	901	-	-	8/20/24/24	0/4/4/4
3	A1AAB	B	901	-	-	6/20/24/24	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	A1AAB	C1-C2	4.02	1.40	1.38
3	D	901	A1AAB	C1-C2	3.72	1.40	1.38
3	B	901	A1AAB	C1-C2	3.68	1.40	1.38
3	A	901	A1AAB	C1-C2	3.51	1.39	1.38
3	B	901	A1AAB	C13-N5	3.34	1.48	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	901	A1AAB	C18-C16-C13	2.94	130.18	121.00
3	A	901	A1AAB	C18-C16-C13	2.64	129.26	121.00
3	D	901	A1AAB	C18-C16-C13	2.50	128.80	121.00

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	901	A1AAB	C13-C16-C18-F2
3	C	901	A1AAB	C13-C16-C18-F2
3	C	901	A1AAB	C13-C16-C18-F
3	C	901	A1AAB	C13-C16-C18-F1
3	B	901	A1AAB	C13-C16-C18-F
3	B	901	A1AAB	C13-C16-C18-F1
3	B	901	A1AAB	C17-C16-C18-F
3	A	901	A1AAB	C13-C16-C18-F1
3	A	901	A1AAB	C13-C16-C18-F
3	A	901	A1AAB	C13-C16-C18-F2
3	D	901	A1AAB	C13-C16-C18-F2
3	D	901	A1AAB	C13-C16-C18-F
3	D	901	A1AAB	C13-C16-C18-F1
3	B	901	A1AAB	C17-C16-C18-F1
3	B	901	A1AAB	C17-C16-C18-F2
3	A	901	A1AAB	C10-C8-O1-C9
3	C	901	A1AAB	C17-C16-C18-F
3	C	901	A1AAB	C17-C16-C18-F2
3	C	901	A1AAB	C17-C16-C18-F1
3	D	901	A1AAB	C3-C2-C8-O1
3	A	901	A1AAB	C17-C16-C18-F
3	A	901	A1AAB	C17-C16-C18-F1
3	A	901	A1AAB	C17-C16-C18-F2
3	A	901	A1AAB	C2-C8-O1-C9

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Mol	Chain	Res	Type	Atoms
3	D	901	A1AAB	C1-C2-C8-O1

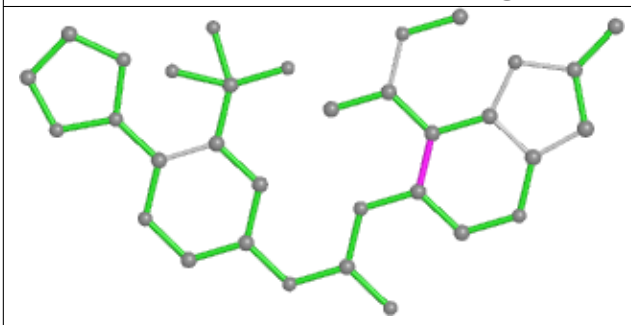
There are no ring outliers.

2 monomers are involved in 5 short contacts:

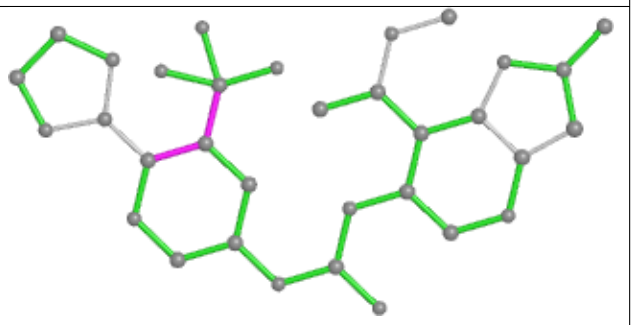
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	901	A1AAB	1	0
3	C	901	A1AAB	4	0

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

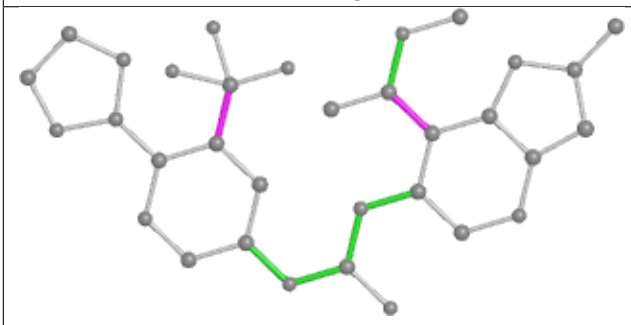
Ligand A1AAB D 901



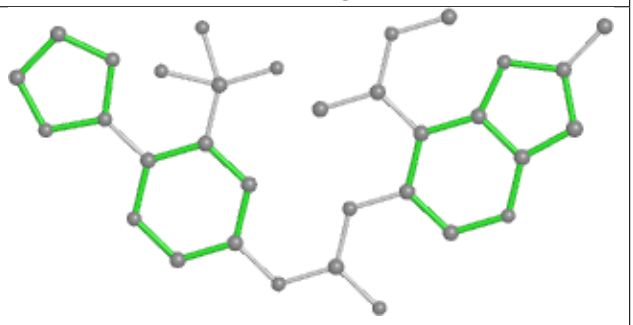
Bond lengths



Bond angles

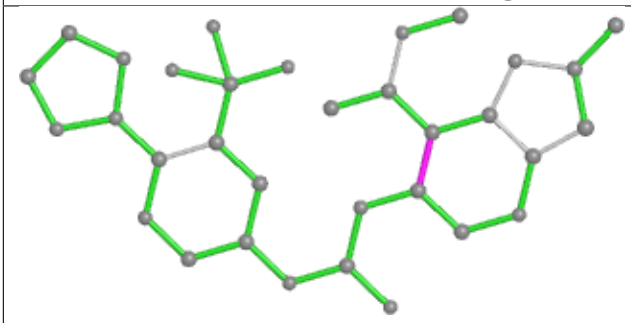


Torsions

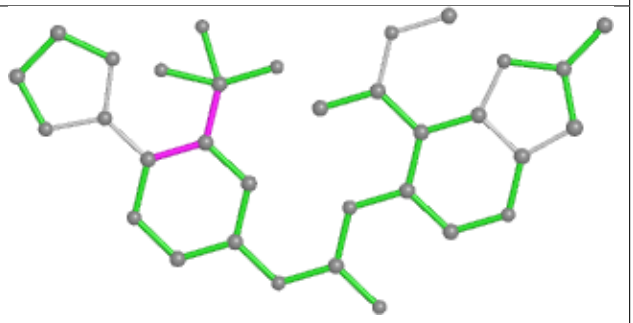


Rings

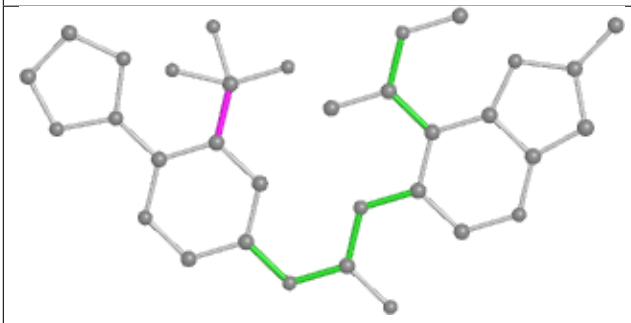
Ligand A1AAB C 901



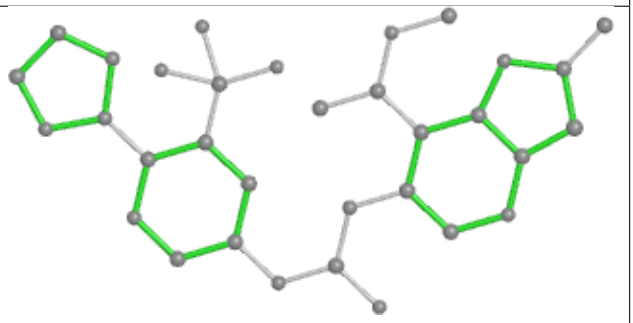
Bond lengths



Bond angles

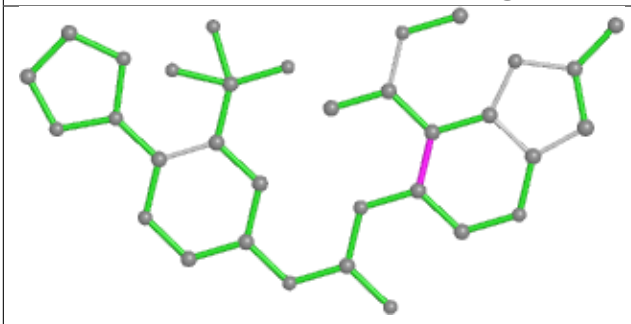


Torsions

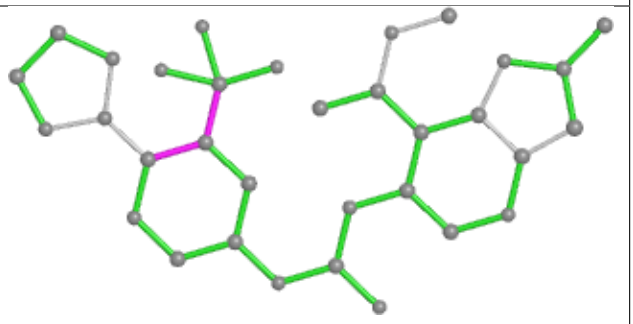


Rings

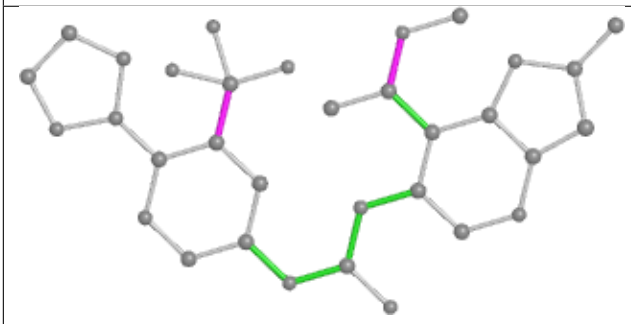
Ligand A1AAB A 901



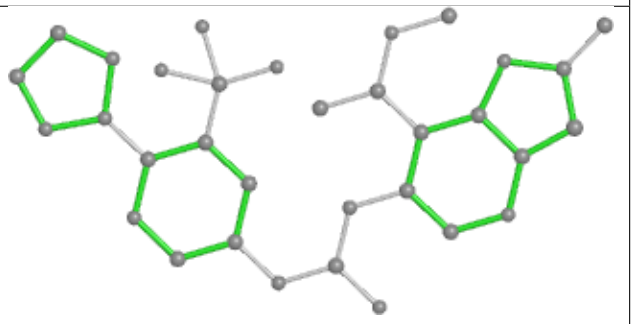
Bond lengths



Bond angles

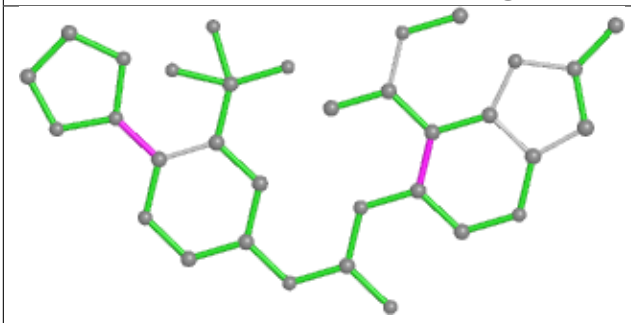


Torsions

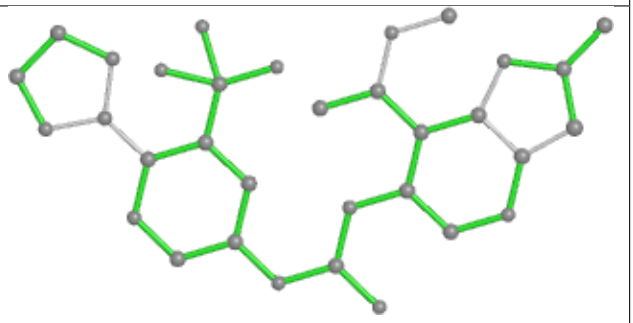


Rings

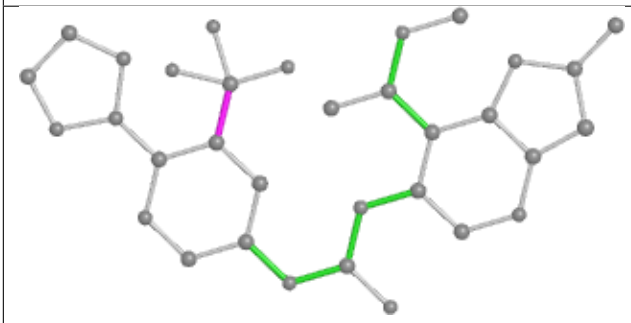
Ligand A1AAB B 901



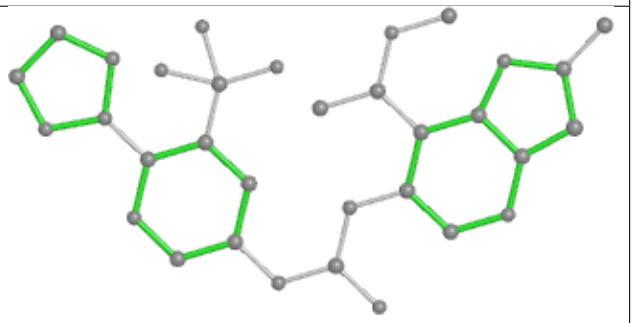
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	367/387 (94%)	-0.10	6 (1%) 72 73	14, 40, 64, 70	0
1	B	360/387 (93%)	-0.18	4 (1%) 80 82	17, 39, 60, 67	0
1	C	361/387 (93%)	0.10	13 (3%) 42 45	20, 47, 75, 83	0
1	D	368/387 (95%)	-0.10	5 (1%) 75 77	15, 46, 69, 76	0
1	E	367/387 (94%)	-0.12	7 (1%) 66 68	17, 43, 64, 88	0
1	F	358/387 (92%)	-0.05	8 (2%) 62 64	20, 45, 64, 78	0
2	G	4/6 (66%)	-0.26	0 100 100	37, 40, 46, 47	0
2	H	4/6 (66%)	-0.16	0 100 100	36, 43, 51, 55	0
2	I	4/6 (66%)	0.47	0 100 100	50, 56, 63, 65	0
2	J	4/6 (66%)	0.17	0 100 100	53, 57, 60, 63	0
2	K	4/6 (66%)	0.24	0 100 100	36, 37, 41, 42	0
2	L	4/6 (66%)	-0.03	0 100 100	38, 42, 47, 49	0
All	All	2205/2358 (93%)	-0.07	43 (1%) 65 67	14, 43, 69, 88	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	573	SER	4.1
1	C	626	ILE	3.8
1	D	623	PRO	3.5
1	C	504	SER	3.5
1	D	470	TYR	3.3
1	F	472	ASP	3.3
1	F	473	THR	3.1
1	C	690	TYR	3.1
1	F	469	ASP	3.0
1	F	565	GLN	3.0
1	E	565	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	432	ASN	3.0
1	C	625	ILE	3.0
1	E	637	LEU	3.0
1	D	622	PRO	2.9
1	C	617	SER	2.8
1	A	619	VAL	2.7
1	E	470	TYR	2.7
1	C	473	THR	2.7
1	B	541	LEU	2.7
1	C	590	MET	2.7
1	C	623	PRO	2.6
1	B	489	GLY	2.6
1	E	433	PRO	2.5
1	A	476	ILE	2.5
1	A	503	HIS	2.5
1	D	626	ILE	2.5
1	F	487	VAL	2.5
1	E	472	ASP	2.4
1	A	489	GLY	2.4
1	B	476	ILE	2.3
1	B	566	GLY	2.3
1	C	646	ALA	2.2
1	A	491	ALA	2.2
1	E	337	GLN	2.2
1	C	600	ILE	2.1
1	D	550	ILE	2.1
1	C	541	LEU	2.1
1	C	692	TYR	2.1
1	C	669	TYR	2.1
1	A	696	GLU	2.1
1	F	461	LEU	2.1
1	F	575	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

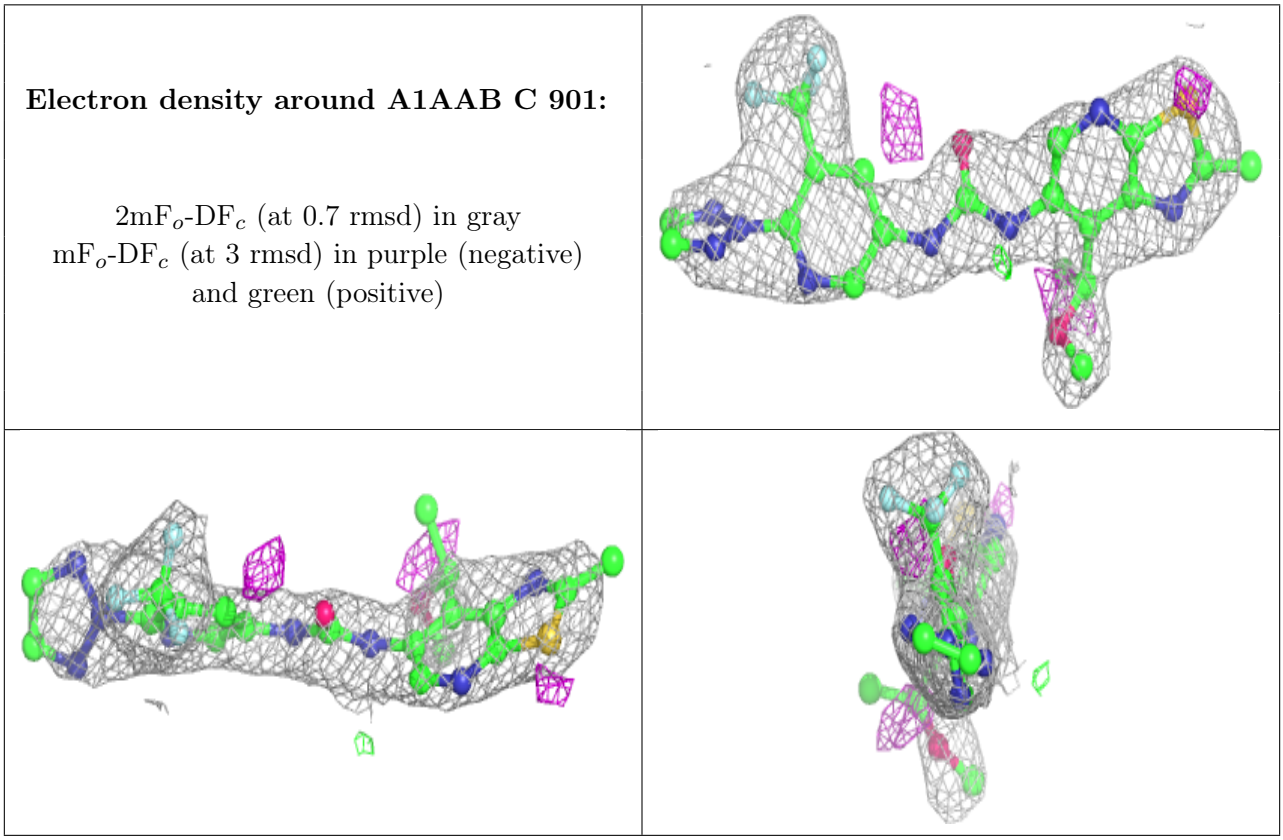
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1AAB	C	901	33/33	0.90	0.25	73,76,77,78	0
3	A1AAB	D	901	33/33	0.96	0.15	63,64,65,65	0
3	A1AAB	A	901	33/33	0.97	0.12	23,24,25,25	0
3	A1AAB	B	901	33/33	0.97	0.12	21,22,24,25	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.

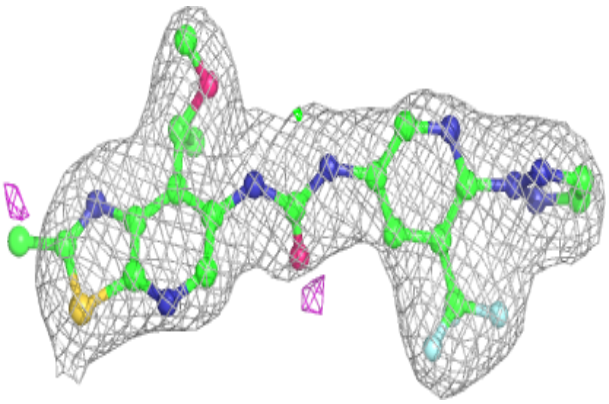
Electron density around A1AAB C 901:

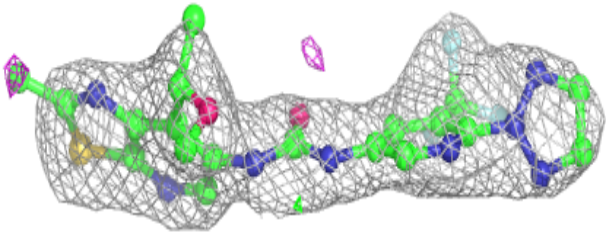
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

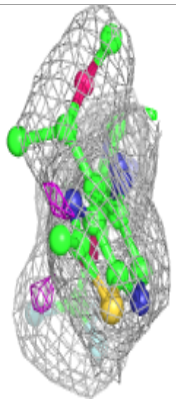


Electron density around A1AAB D 901:

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

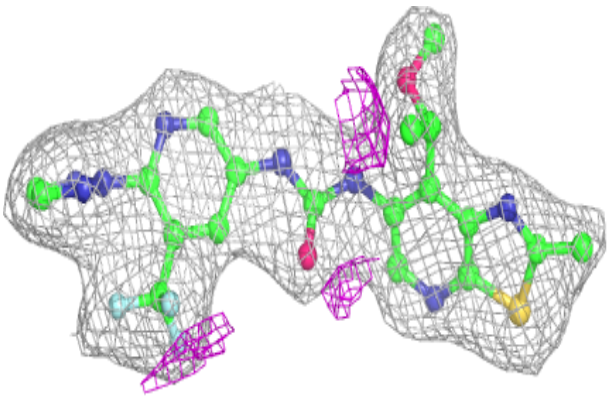


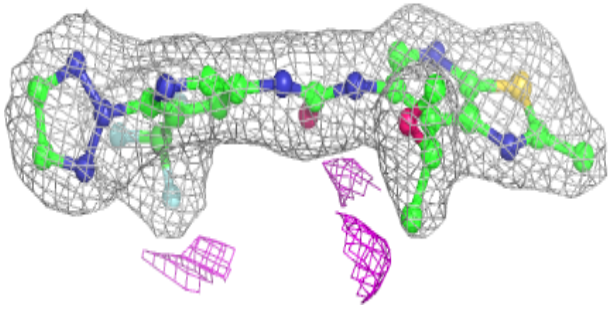


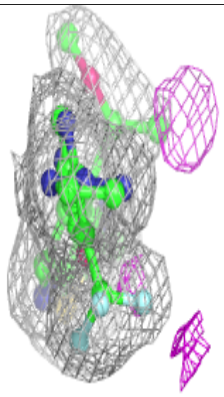


Electron density around A1AAB A 901:

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

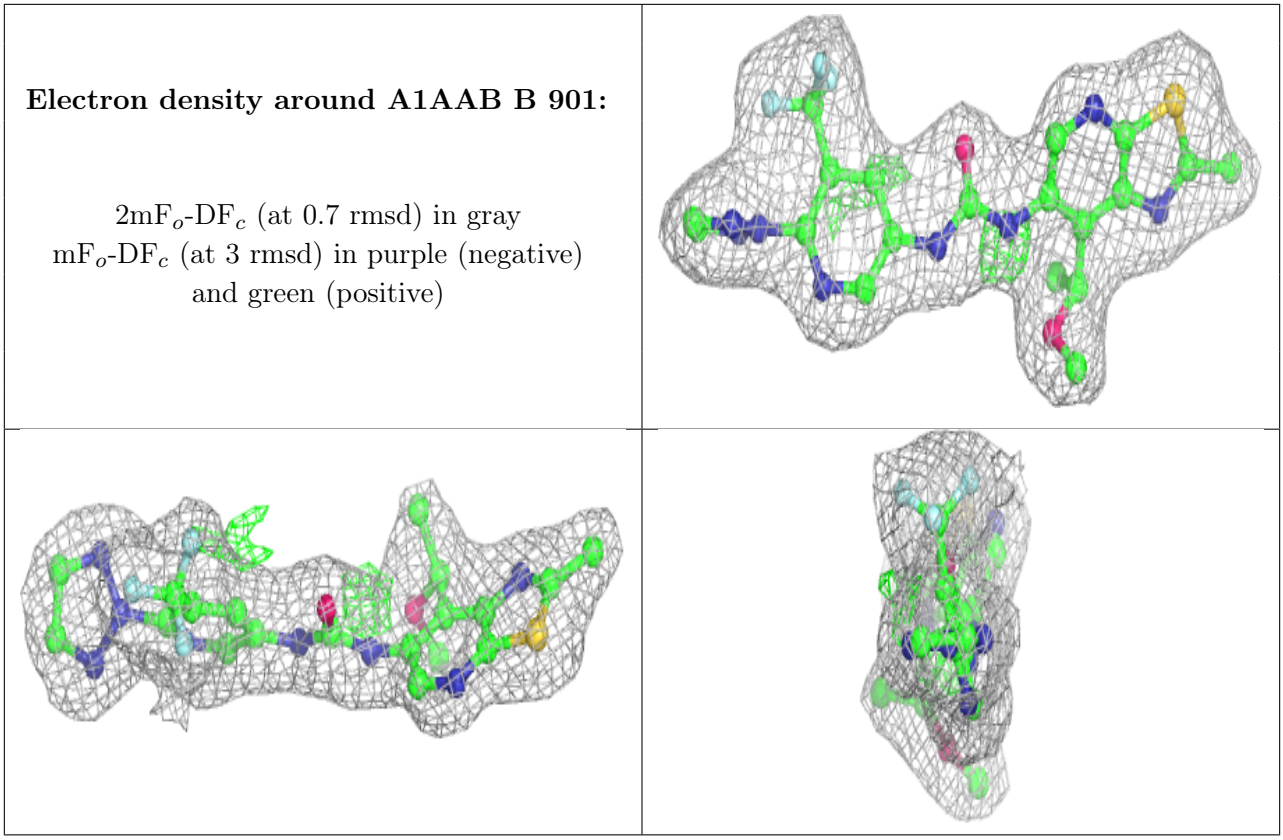






Electron density around A1AAB B 901:

$2mF_o$-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.