



Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2026 – 11:16 pm BST

PDB ID : 9R5N / pdb_00009r5n
Title : FKBP12 in complex with binfunctional ligand b3c and the first bromodomain of BRD4
Authors : Meyners, C.; Hausch, F.
Deposited on : 2025-05-09
Resolution : 3.00 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	:	1.8.4, CSD as541be (2020)
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

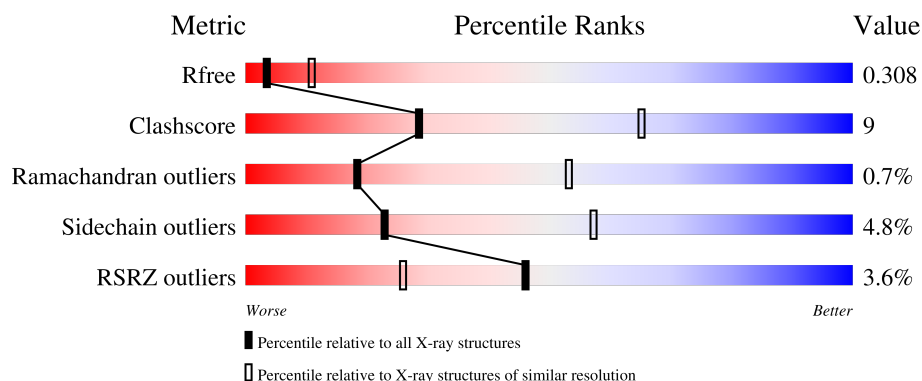
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	127	<div> <div>2%</div> <div>54%</div> <div>26%</div> <div>17%</div> </div>
1	B	127	<div> <div>8%</div> <div>55%</div> <div>22%</div> <div>20%</div> </div>
2	C	107	<div> <div>%</div> <div>52%</div> <div>37%</div> <div>10%</div> </div>
2	D	107	<div> <div>%</div> <div>66%</div> <div>28%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6709 atoms, of which 3296 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 Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	105	Total	C	H	N	O	S	35	0	0
			1687	559	830	139	153	6			
1	B	102	Total	C	H	N	O	S	47	0	0
			1588	534	782	124	142	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O60885
A	1	MET	-	expression tag	UNP O60885
B	0	SER	-	expression tag	UNP O60885
B	1	MET	-	expression tag	UNP O60885

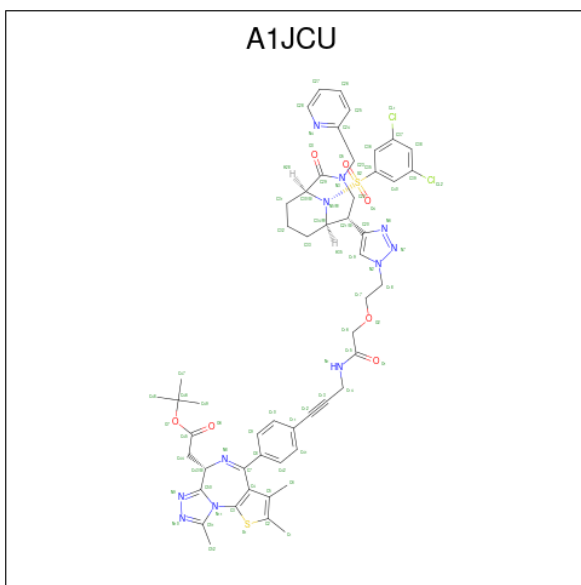
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	107	Total	C	H	N	O	S	35	0	0
			1588	510	787	136	152	3			
2	D	107	Total	C	H	N	O	S	35	0	0
			1588	510	787	136	152	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	22	VAL	CYS	engineered mutation	UNP P62942
D	22	VAL	CYS	engineered mutation	UNP P62942

- Molecule 3 is {tert}-butyl 2-[(9 {S})-7-[4-[3-[2-[2-[4-[(1 {S}),5 {S}),6 {R})-10-[3,5-bis(chloranyl)phenyl]sulfonyl-2-oxidanylidene-3-(pyridin-2-ylmethyl)-3,10-diazabicyclo[4.3.1]decan-5-yl]-1,2,3-triazol-1-yl]ethoxy]ethanoylamino]prop-1-ynyl]phenyl]-4,5,13-trimethyl-3-thia-1,8,11,12-tetrazatricyclo[8.3.0.0[^]{2,6}]trideca-2(6),4,7,10,12-pentaen-9-yl]ethanoate (CCD ID: A1JCU) (formula: C₅₂H₅₅Cl₂N₁₁O₇S₂) (labeled as "Ligand of Interest" by depositor).

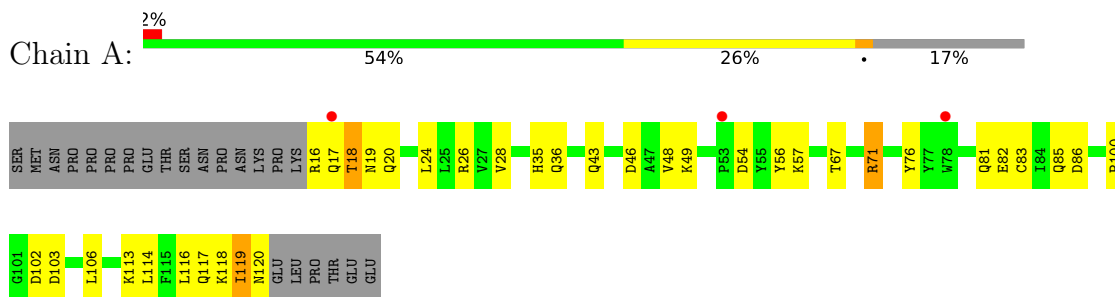


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total 129	C 52	Cl 2	H 55	N 11	O 7	S 2	9	0
3	B	1	Total 129	C 52	Cl 2	H 55	N 11	O 7	S 2	9	0

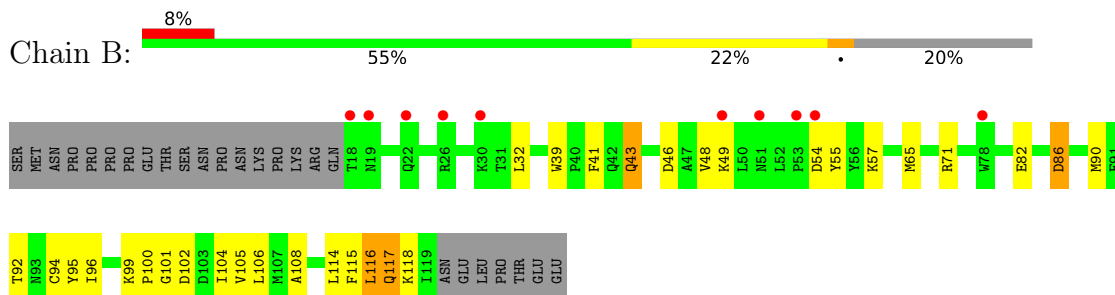
3 Residue-property plots [i](#)

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.

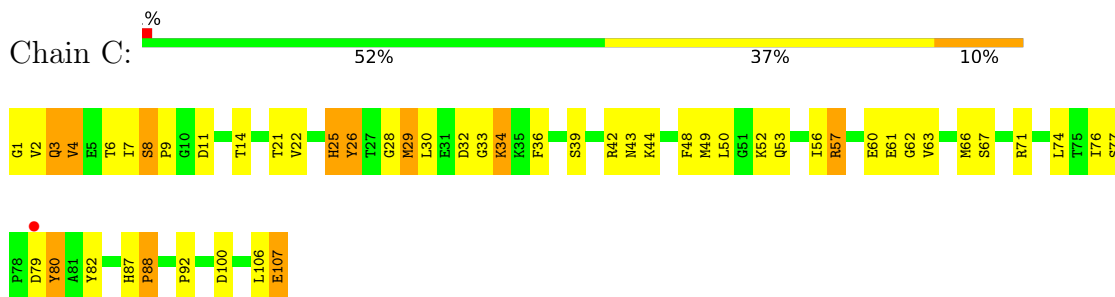
- Molecule 1: Bromodomain-containing protein 4



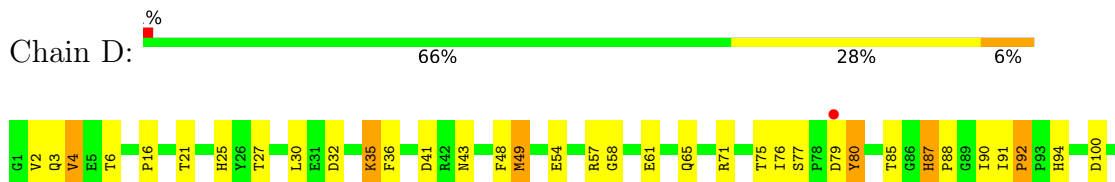
- Molecule 1: Bromodomain-containing protein 4



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.82Å 90.51Å 103.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 3.00 48.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.72-3.00) 99.8 (48.72-3.00)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.260 , 0.312 0.255 , 0.308	Depositor DCC
R_{free} test set	597 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	1.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6709	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 48.17 % 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 8.9433e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1JCU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	1/880 (0.1%)	1.69	16/1203 (1.3%)
1	B	1.07	0/829	1.75	16/1137 (1.4%)
2	C	1.29	3/820 (0.4%)	1.81	25/1112 (2.2%)
2	D	1.29	2/820 (0.2%)	1.83	17/1112 (1.5%)
All	All	1.18	6/3349 (0.2%)	1.77	74/4564 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	C	0	1
2	D	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	67	SER	CA-CB	-6.36	1.43	1.53
2	C	25	HIS	CG-CD2	-5.88	1.29	1.35
2	D	4	VAL	C-O	-5.68	1.18	1.24
2	C	107	GLU	CD-OE1	5.56	1.35	1.25
1	A	100	PRO	C-N	-5.46	1.28	1.34
2	D	87	HIS	CG-CD2	-5.17	1.30	1.35

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	LYS	N-CA-CB	11.20	127.47	110.22
1	B	46	ASP	CB-CA-C	9.57	127.76	111.68
1	A	49	LYS	N-CA-CB	9.32	124.04	110.06
2	D	92	PRO	CA-C-N	8.32	128.84	119.93
2	D	92	PRO	C-N-CA	8.32	128.84	119.93
1	B	116	LEU	N-CA-C	-8.25	102.24	111.07
2	C	3	GLN	N-CA-CB	8.20	124.07	110.47
1	B	118	LYS	N-CA-CB	-7.76	97.37	110.41
1	A	67	THR	CA-CB-OG1	-7.73	98.00	109.60
1	A	82	GLU	N-CA-CB	-7.70	98.79	110.33
2	D	100	ASP	CB-CA-C	7.65	123.02	110.78
1	B	43	GLN	O-C-N	-7.28	117.05	121.71
2	D	6	THR	CA-CB-OG1	-7.20	98.80	109.60
2	D	54	GLU	CG-CD-OE1	-7.02	102.26	118.40
2	D	80	TYR	N-CA-C	-7.01	104.60	113.72
1	A	17	GLN	N-CA-CB	-6.98	100.96	111.64
2	C	57	ARG	NH1-CZ-NH2	6.88	128.24	119.30
2	D	36	PHE	CA-CB-CG	6.88	120.67	113.80
2	D	54	GLU	N-CA-C	-6.68	104.71	112.92
1	B	82	GLU	N-CA-CB	-6.59	100.44	110.33
1	B	54	ASP	CB-CA-C	6.54	122.82	109.55
2	C	36	PHE	N-CA-C	-6.51	105.97	114.04
1	A	100	PRO	CA-C-N	-6.47	116.44	123.30
1	A	100	PRO	C-N-CA	-6.47	116.44	123.30
2	C	11	ASP	CA-CB-CG	6.39	118.99	112.60
2	C	34	LYS	CB-CA-C	6.38	117.64	109.80
1	B	117	GLN	CB-CA-C	6.36	121.29	110.74
1	A	54	ASP	CB-CA-C	6.32	121.85	109.72
1	A	57	LYS	N-CA-C	-6.10	104.75	111.82
1	B	118	LYS	N-CA-C	6.08	120.54	113.18
1	A	102	ASP	CA-CB-CG	5.97	118.57	112.60
2	C	43	ASN	CA-CB-CG	-5.92	106.68	112.60
2	C	52	LYS	CB-CA-C	5.91	119.97	110.09
1	A	46	ASP	CA-CB-CG	5.75	118.35	112.60
2	D	48	PHE	CA-CB-CG	5.74	119.54	113.80
2	D	35	LYS	CB-CA-C	5.67	119.89	109.46
1	B	118	LYS	CB-CA-C	5.67	121.22	109.95
2	C	53	GLN	N-CA-CB	5.65	120.06	111.70
1	A	36	GLN	CB-CA-C	-5.65	98.72	109.95
2	C	14	THR	CA-CB-CG2	5.61	120.03	110.50
2	C	53	GLN	CB-CA-C	-5.59	103.94	111.89
2	C	26	TYR	N-CA-CB	-5.56	102.19	111.20
2	D	49	MET	CG-SD-CE	-5.55	88.68	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	ILE	N-CA-C	-5.55	106.40	111.67
2	C	6	THR	CA-CB-OG1	-5.52	101.32	109.60
2	C	36	PHE	CB-CA-C	5.50	118.94	109.15
1	B	101	GLY	CA-C-O	5.48	124.88	118.96
1	A	43	GLN	O-C-N	-5.47	118.21	121.71
2	C	8	SER	CA-C-N	5.47	126.67	119.84
2	C	8	SER	C-N-CA	5.47	126.67	119.84
1	A	83	CYS	N-CA-C	-5.42	105.28	111.14
2	C	80	TYR	N-CA-CB	-5.41	102.35	110.73
2	D	43	ASN	CB-CA-C	5.39	119.68	111.80
2	C	4	VAL	N-CA-CB	-5.37	105.16	111.39
2	D	16	PRO	N-CA-CB	-5.34	98.37	103.34
2	C	36	PHE	CA-CB-CG	5.33	119.13	113.80
2	C	39	SER	N-CA-C	-5.33	106.62	113.23
1	A	85	GLN	CB-CA-C	-5.29	102.35	110.81
2	D	105	LYS	N-CA-CB	5.26	119.88	111.56
1	A	18	THR	CA-CB-OG1	-5.25	101.72	109.60
2	D	77	SER	CA-C-N	5.21	126.36	119.84
2	D	77	SER	C-N-CA	5.21	126.36	119.84
1	B	49	LYS	CB-CA-C	-5.19	101.03	110.63
2	C	71	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	B	102	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	100	PRO	N-CA-CB	-5.17	98.53	103.34
2	D	3	GLN	N-CA-CB	5.17	118.89	110.37
2	C	92	PRO	CA-C-N	5.15	125.39	119.83
2	C	92	PRO	C-N-CA	5.15	125.39	119.83
1	A	76	TYR	N-CA-CB	-5.10	101.84	110.41
2	C	82	TYR	CB-CA-C	5.09	117.96	109.56
1	B	86	ASP	CA-CB-CG	5.08	117.68	112.60
2	C	48	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	115	PHE	N-CA-CB	-5.04	102.71	110.01

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ARG	Sidechain
1	A	26	ARG	Sidechain
1	A	71	ARG	Sidechain
2	C	42	ARG	Sidechain
2	D	71	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	857	830	810	14	0
1	B	806	782	750	14	0
2	C	801	787	770	21	0
2	D	801	787	770	11	0
3	A	74	55	0	1	0
3	B	74	55	0	0	0
All	All	3413	3296	3100	57	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 9.

All (57) 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:18:THR:HG22	1:A:20:GLN:H	1.42	0.84
2:D:35:LYS:NZ	2:D:41:ASP:OD2	2.15	0.79
2:C:4:VAL:HG22	2:C:74:LEU:HD22	1.64	0.78
1:A:48:VAL:HG12	2:D:61:GLU:OE2	1.84	0.76
1:B:32:LEU:HB3	1:B:65:MET:HE1	1.70	0.73
1:A:116:LEU:HD23	1:A:119:ILE:HD11	1.75	0.68
1:A:116:LEU:HA	1:A:119:ILE:HG12	1.80	0.63
2:C:79:ASP:OD1	2:C:80:TYR:HD1	1.84	0.60
2:C:57:ARG:HG2	2:C:80:TYR:CD2	2.39	0.58
1:B:32:LEU:HB3	1:B:65:MET:CE	2.34	0.56
2:C:22:VAL:HG22	2:C:106:LEU:CD2	2.38	0.54
1:A:18:THR:HG22	1:A:20:GLN:N	2.18	0.53
1:B:116:LEU:O	1:B:117:GLN:C	2.51	0.53
1:B:94:CYS:SG	1:B:104:ILE:HG13	2.49	0.52
2:C:21:THR:N	2:C:107:GLU:O	2.42	0.52
1:B:71:ARG:NH1	1:B:86:ASP:OD2	2.44	0.51
2:D:79:ASP:OD1	2:D:80:TYR:HD1	1.95	0.50
1:B:48:VAL:HB	2:C:61:GLU:OE2	2.12	0.49
2:D:30:LEU:HB2	2:D:32:ASP:OD1	2.12	0.48
1:A:118:LYS:C	1:A:120:ASN:H	2.21	0.48
2:C:33:GLY:O	2:C:34:LYS:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD22	3:A:201:A1JCU:C27	2.43	0.48
2:C:63:VAL:O	2:C:66:MET:HB2	2.13	0.47
1:A:35:HIS:HD2	1:A:114:LEU:HD22	1.79	0.47
2:C:22:VAL:HG22	2:C:106:LEU:HD23	1.96	0.47
2:C:28:GLY:C	2:C:29:MET:HG3	2.39	0.47
2:C:30:LEU:C	2:C:32:ASP:H	2.22	0.47
2:C:49:MET:HE3	2:C:49:MET:HB2	1.32	0.47
2:C:50:LEU:HD12	2:C:60:GLU:HG2	1.97	0.46
1:B:41:PHE:CZ	1:B:108:ALA:HB2	2.51	0.46
2:D:58:GLY:HA3	2:D:76:ILE:HG12	1.98	0.45
1:A:71:ARG:NH1	1:A:86:ASP:OD2	2.50	0.45
2:C:87:HIS:O	2:C:88:PRO:C	2.60	0.45
2:C:2:VAL:HG23	2:C:76:ILE:HG12	1.99	0.44
2:D:49:MET:HE3	2:D:49:MET:HB2	1.72	0.44
2:D:57:ARG:HG2	2:D:80:TYR:CD2	2.53	0.43
1:A:24:LEU:HD23	1:A:28:VAL:HG21	2.01	0.43
1:B:39:TRP:O	1:B:43:GLN:NE2	2.52	0.43
2:C:87:HIS:HA	2:C:88:PRO:HD2	1.84	0.42
2:C:1:GLY:HA2	2:C:77:SER:OG	2.18	0.42
1:B:65:MET:HG3	1:B:90:MET:SD	2.59	0.42
1:A:56:TYR:CD1	2:D:65:GLN:HG2	2.55	0.42
1:B:114:LEU:O	1:B:117:GLN:HB3	2.19	0.42
1:A:117:GLN:O	1:A:120:ASN:HB3	2.19	0.42
2:C:26:TYR:HA	2:C:100:ASP:O	2.20	0.42
1:A:18:THR:HG22	1:A:19:ASN:N	2.35	0.42
2:C:30:LEU:C	2:C:32:ASP:N	2.78	0.42
1:A:116:LEU:HA	1:A:119:ILE:CG1	2.49	0.42
2:C:8:SER:HA	2:C:9:PRO:HD2	1.82	0.41
2:D:2:VAL:HA	2:D:75:THR:O	2.20	0.41
1:B:55:TYR:C	1:B:57:LYS:N	2.78	0.41
1:B:92:THR:O	1:B:96:ILE:HG13	2.20	0.41
2:D:91:ILE:HA	2:D:92:PRO:HD3	1.94	0.41
2:D:87:HIS:HA	2:D:88:PRO:HD2	1.81	0.41
1:B:95:TYR:CD1	1:B:105:VAL:HG13	2.57	0.40
2:C:56:ILE:HD13	2:C:56:ILE:HG21	1.93	0.40
1:B:65:MET:CG	1:B:90:MET:HE1	2.51	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	103/127 (81%)	98 (95%)	4 (4%)	1 (1%)	12	45
1	B	100/127 (79%)	95 (95%)	5 (5%)	0	100	100
2	C	105/107 (98%)	95 (90%)	8 (8%)	2 (2%)	6	30
2	D	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
All	All	413/468 (88%)	386 (94%)	24 (6%)	3 (1%)	18	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	62	GLY
2	C	88	PRO
1	A	119	ILE

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	89/120 (74%)	86 (97%)	3 (3%)	32	66
1	B	80/120 (67%)	78 (98%)	2 (2%)	42	72
2	C	82/89 (92%)	78 (95%)	4 (5%)	22	56
2	D	82/89 (92%)	75 (92%)	7 (8%)	10	36
All	All	333/418 (80%)	317 (95%)	16 (5%)	23	57

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	103	ASP
1	A	113	LYS
1	B	99	LYS
1	B	106	LEU
2	C	3	GLN
2	C	25	HIS
2	C	29	MET
2	C	44	LYS
2	D	4	VAL
2	D	21	THR
2	D	25	HIS
2	D	27	THR
2	D	85	THR
2	D	90	ILE
2	D	94	HIS

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

Mol	Chain	Res	Type
1	A	74	ASN
1	A	79	ASN
1	A	88	ASN
1	A	98	ASN
1	B	81	GLN
2	C	25	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	A1JCU	A	201	-	74,82,82	1.41	9 (12%)	91,121,121	1.95	21 (23%)
3	A1JCU	B	201	-	74,82,82	1.42	10 (13%)	91,121,121	2.30	29 (31%)

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	A1JCU	A	201	-	-	12/41/93/93	0/7/9/9
3	A1JCU	B	201	-	-	11/41/93/93	0/7/9/9

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	A1JCU	C29-N3	-5.27	1.29	1.35
3	A	201	A1JCU	C50-N9	-4.51	1.27	1.32
3	B	201	A1JCU	C30-C29	-3.41	1.49	1.53
3	A	201	A1JCU	C4-C3	3.40	1.45	1.39
3	B	201	A1JCU	C4-C3	3.14	1.45	1.39
3	B	201	A1JCU	C50-N9	-3.13	1.28	1.32
3	A	201	A1JCU	C30-C29	-3.02	1.49	1.53
3	A	201	A1JCU	C35-S2	-2.81	1.72	1.76
3	B	201	A1JCU	O2-C16	2.65	1.48	1.42
3	A	201	A1JCU	O2-C16	2.64	1.48	1.42
3	B	201	A1JCU	O7-C46	2.51	1.53	1.48
3	A	201	A1JCU	C29-N3	-2.48	1.32	1.35
3	B	201	A1JCU	C30-N5	-2.34	1.46	1.48
3	B	201	A1JCU	O6-C45	2.33	1.29	1.22
3	A	201	A1JCU	C19-N2	-2.26	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	A1JCU	O1-C15	-2.25	1.18	1.23
3	B	201	A1JCU	C4-C5	2.24	1.50	1.42
3	A	201	A1JCU	C39-CL2	-2.18	1.69	1.74
3	B	201	A1JCU	C51-N10	-2.09	1.28	1.31

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	A1JCU	C43-N8-C7	8.53	125.72	117.62
3	A	201	A1JCU	C43-N8-C7	7.75	124.99	117.62
3	B	201	A1JCU	C22-N3-C29	6.61	130.49	122.37
3	B	201	A1JCU	C1-C2-C5	6.03	142.59	128.59
3	B	201	A1JCU	C50-C43-N8	5.81	116.19	106.72
3	B	201	A1JCU	O5-S2-O4	-4.89	111.60	119.52
3	A	201	A1JCU	C1-C2-C5	4.67	139.43	128.59
3	A	201	A1JCU	C13-C14-N1	4.52	118.34	112.71
3	A	201	A1JCU	C20-N6-N7	-4.34	105.64	109.24
3	B	201	A1JCU	C40-C35-S2	4.27	124.10	119.34
3	A	201	A1JCU	C44-C43-N8	4.23	115.16	109.82
3	B	201	A1JCU	C8-C7-N8	4.13	122.00	117.27
3	B	201	A1JCU	C35-S2-N5	-4.01	94.76	106.43
3	A	201	A1JCU	C50-C43-N8	3.88	113.06	106.72
3	A	201	A1JCU	O5-S2-C35	3.85	112.92	108.05
3	A	201	A1JCU	N11-C51-N10	-3.76	105.69	109.60
3	B	201	A1JCU	C6-C5-C4	-3.69	115.97	125.93
3	B	201	A1JCU	O4-S2-N5	3.54	114.27	107.13
3	A	201	A1JCU	O3-C29-N3	-3.46	119.26	122.55
3	B	201	A1JCU	O5-S2-N5	3.35	113.89	107.13
3	B	201	A1JCU	C46-O7-C45	3.31	128.60	121.79
3	B	201	A1JCU	C24-C23-N3	-3.27	108.11	113.65
3	A	201	A1JCU	C4-C5-C2	3.27	118.36	111.91
3	B	201	A1JCU	O3-C29-N3	-3.23	119.47	122.55
3	B	201	A1JCU	C37-C36-C35	3.14	121.05	118.23
3	A	201	A1JCU	C51-N11-C50	3.12	107.88	105.08
3	A	201	A1JCU	C6-C5-C4	-3.09	117.57	125.93
3	B	201	A1JCU	C1-C2-S1	-3.06	110.81	118.27
3	B	201	A1JCU	C4-C5-C2	2.87	117.56	111.91
3	B	201	A1JCU	C40-C35-C36	-2.86	116.42	120.31
3	A	201	A1JCU	C1-C2-S1	-2.81	111.43	118.27
3	A	201	A1JCU	C51-N10-N9	2.78	110.62	107.89
3	A	201	A1JCU	O4-S2-N5	2.69	112.56	107.13
3	B	201	A1JCU	C39-C40-C35	2.67	120.62	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	A1JCU	C21-C34-N5	2.66	118.01	110.87
3	A	201	A1JCU	C46-O7-C45	2.60	127.15	121.79
3	B	201	A1JCU	C5-C2-S1	-2.55	106.59	111.57
3	B	201	A1JCU	O5-S2-C35	2.55	111.28	108.05
3	B	201	A1JCU	C14-N1-C15	2.50	124.08	121.60
3	A	201	A1JCU	O7-C46-C49	2.46	116.94	107.20
3	A	201	A1JCU	C22-N3-C29	2.42	125.35	122.37
3	B	201	A1JCU	C20-N6-N7	-2.39	107.26	109.24
3	B	201	A1JCU	O2-C16-C15	-2.31	107.43	112.38
3	B	201	A1JCU	C49-C46-C48	2.22	116.99	111.16
3	A	201	A1JCU	C18-N2-C19	-2.14	124.77	128.83
3	B	201	A1JCU	C36-C37-CL1	-2.13	116.49	119.15
3	A	201	A1JCU	C14-N1-C15	2.09	123.67	121.60
3	B	201	A1JCU	C30-N5-S2	2.07	122.97	118.27
3	A	201	A1JCU	C24-C23-N3	-2.03	110.21	113.65
3	B	201	A1JCU	C16-O2-C17	2.00	118.36	113.13

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	A1JCU	C24-C23-N3-C22
3	B	201	A1JCU	C49-C46-O7-C45
3	B	201	A1JCU	C47-C46-O7-C45
3	B	201	A1JCU	C48-C46-O7-C45
3	A	201	A1JCU	C48-C46-O7-C45
3	A	201	A1JCU	C49-C46-O7-C45
3	A	201	A1JCU	C47-C46-O7-C45
3	A	201	A1JCU	C17-C18-N2-N7
3	B	201	A1JCU	C44-C45-O7-C46
3	A	201	A1JCU	C17-C18-N2-C19
3	B	201	A1JCU	C17-C18-N2-C19
3	A	201	A1JCU	O6-C45-O7-C46
3	B	201	A1JCU	O2-C17-C18-N2
3	A	201	A1JCU	C30-N5-S2-O4
3	B	201	A1JCU	C30-N5-S2-O4
3	B	201	A1JCU	O6-C45-O7-C46
3	B	201	A1JCU	C17-C18-N2-N7
3	B	201	A1JCU	C18-C17-O2-C16
3	A	201	A1JCU	N8-C43-C44-C45
3	A	201	A1JCU	C30-N5-S2-C35
3	B	201	A1JCU	C30-N5-S2-C35

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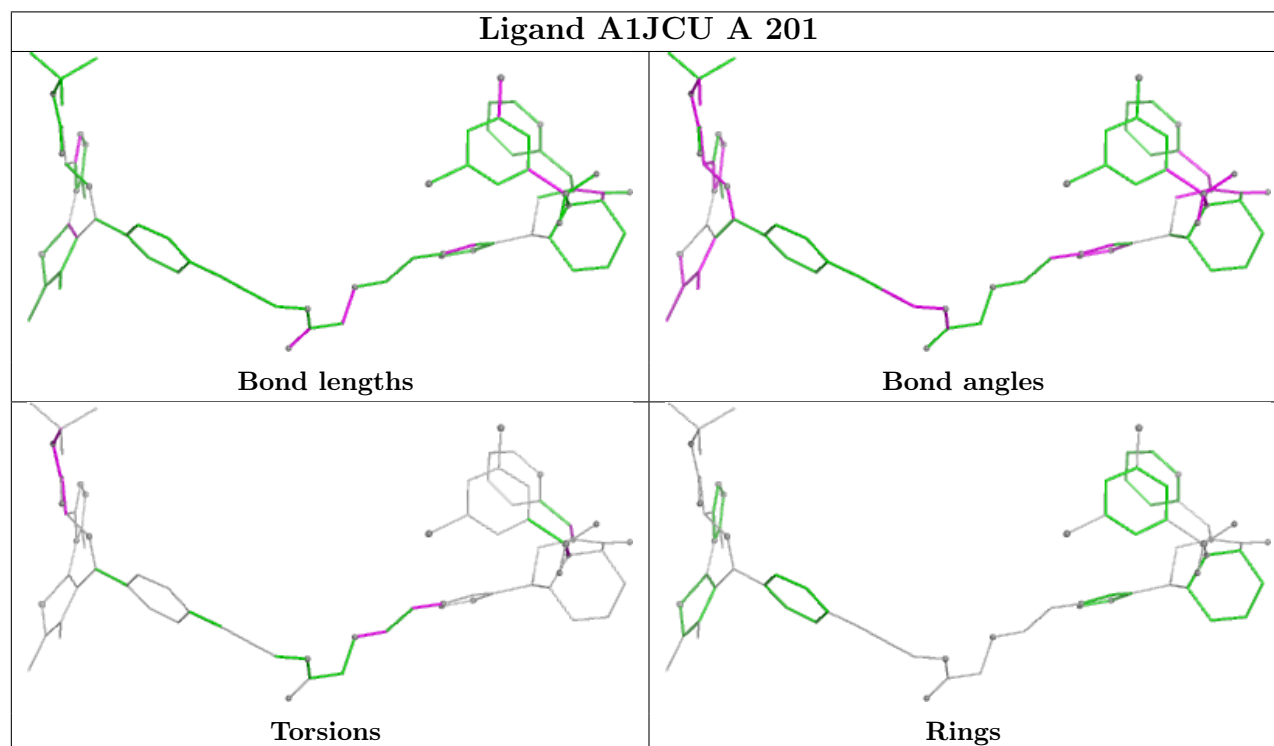
Mol	Chain	Res	Type	Atoms
3	A	201	A1JCU	C44-C45-O7-C46
3	A	201	A1JCU	C18-C17-O2-C16

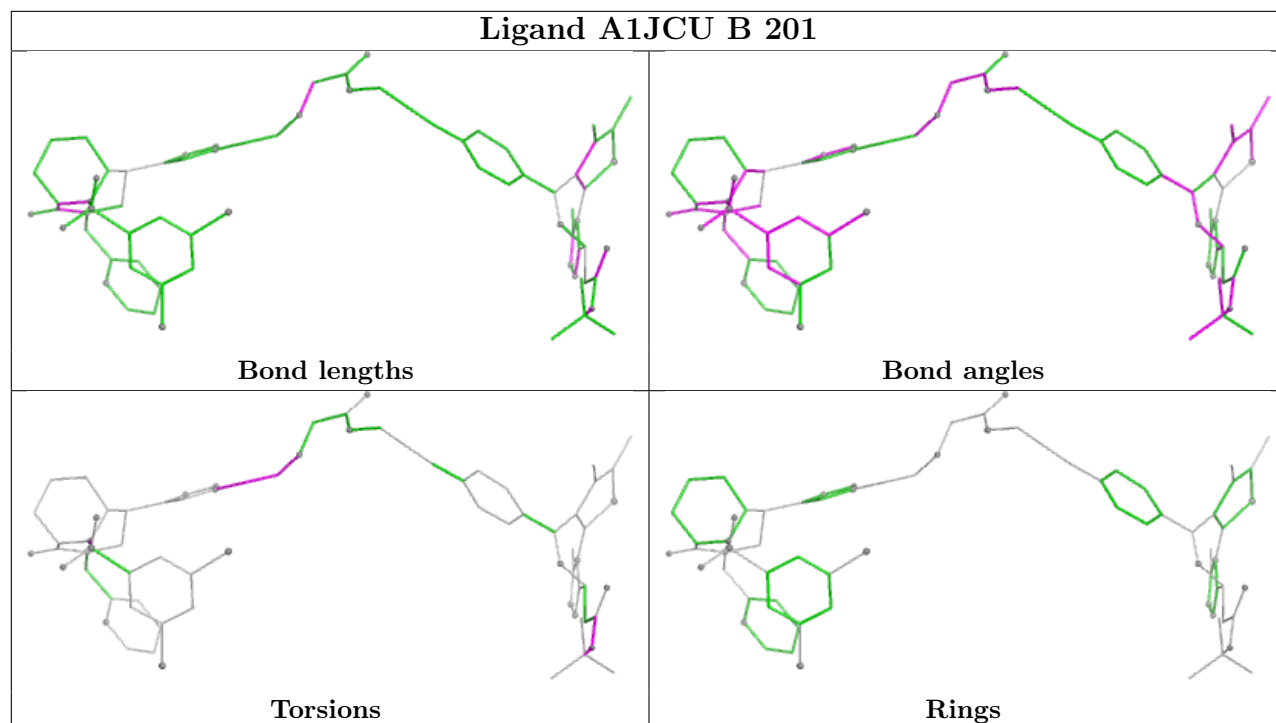
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	A1JCU	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 [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, 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	105/127 (82%)	0.39	3 (2%) 53 31	16, 26, 57, 71	0
1	B	102/127 (80%)	0.57	10 (9%) 13 7	16, 27, 52, 62	0
2	C	107/107 (100%)	0.16	1 (0%) 81 61	14, 22, 34, 42	0
2	D	107/107 (100%)	0.15	1 (0%) 81 61	13, 23, 33, 39	0
All	All	421/468 (89%)	0.31	15 (3%) 46 26	13, 24, 48, 71	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	PRO	4.8
1	A	17	GLN	3.9
1	B	19	ASN	3.3
1	B	51	ASN	3.3
1	B	78	TRP	3.1
1	B	22	GLN	2.9
1	B	54	ASP	2.6
1	A	53	PRO	2.4
1	B	30	LYS	2.4
2	C	79	ASP	2.3
1	B	26	ARG	2.2
2	D	79	ASP	2.2
1	A	78	TRP	2.2
1	B	18	THR	2.1
1	B	49	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

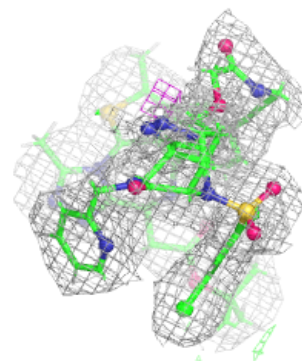
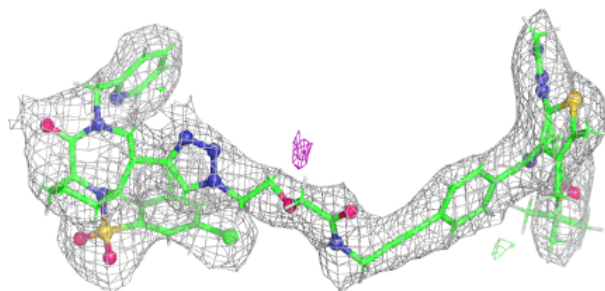
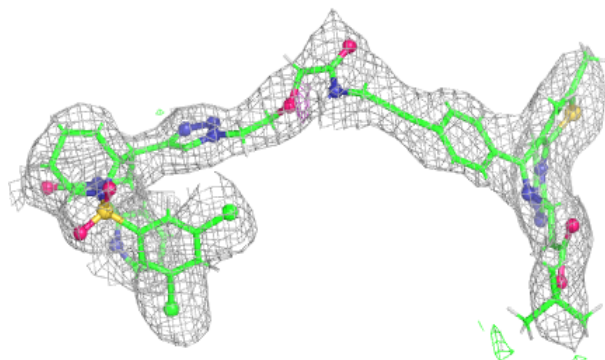
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1JCU	B	201	74/74	0.94	0.10	18,21,30,30	9
3	A1JCU	A	201	74/74	0.95	0.09	18,24,30,30	9

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.

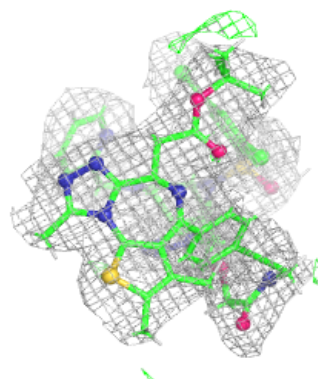
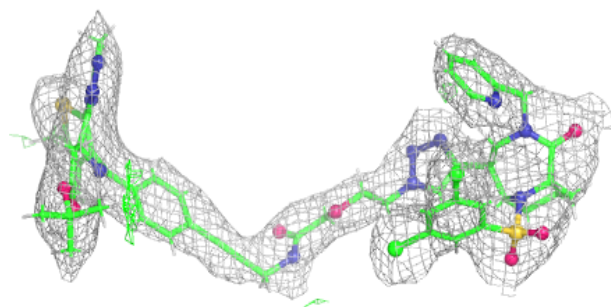
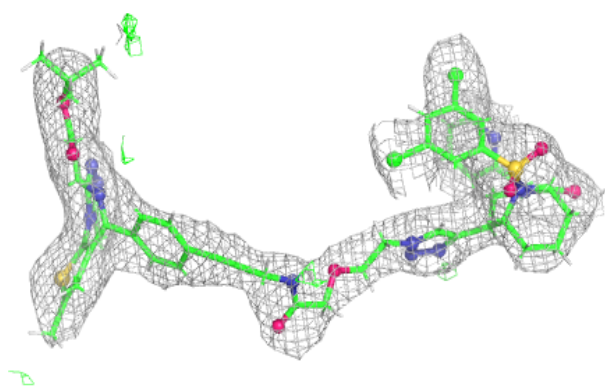
Electron density around A1JCU B 201:

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 A1JCU A 201:

$2mF_o-DF_c$ (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.