



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:14 AM UTC

PDB ID : 3LJ1 / pdb_00003lj1
Title : IRE1 complexed with Cdk1/2 Inhibitor III
Authors : Lee, K.P.K.; Sicheri, F.
Deposited on : 2010-01-25
Resolution : 3.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

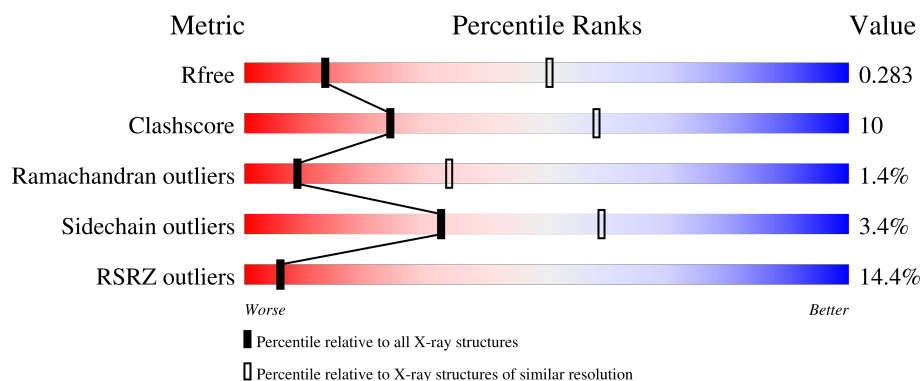
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	434	15% 76% 13% 6%
1	B	434	12% 76% 15% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6348 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	P	S	0	0	0
			3146	2012	535	582	3	14			
1	B	407	Total	C	N	O	P	S	0	0	0
			3146	2012	535	582	3	14			

There are 48 discrepancies between the modelled and reference sequences:

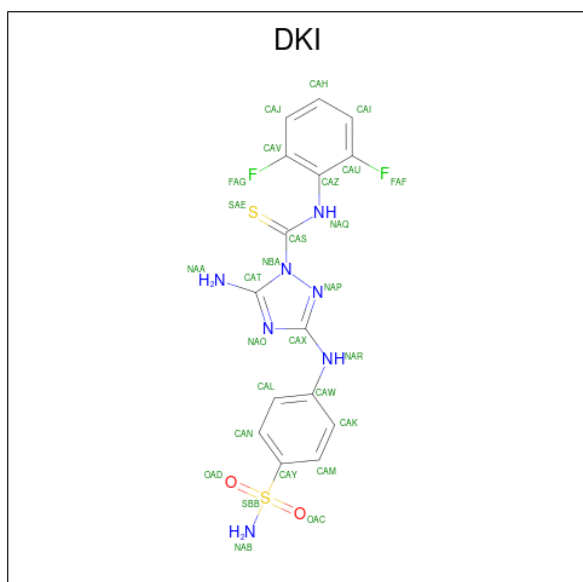
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	deletion	UNP P32361
A	?	-	GLN	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	GLU	deletion	UNP P32361
A	?	-	THR	deletion	UNP P32361
A	?	-	GLU	deletion	UNP P32361
A	?	-	HIS	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	ARG	deletion	UNP P32361
A	?	-	HIS	deletion	UNP P32361
A	?	-	THR	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	ASP	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	PHE	deletion	UNP P32361
A	?	-	TYR	deletion	UNP P32361
A	?	-	ASP	deletion	UNP P32361
A	?	-	PRO	deletion	UNP P32361
A	?	-	PHE	deletion	UNP P32361
B	?	-	CYS	deletion	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	GLU	deletion	UNP P32361
B	?	-	THR	deletion	UNP P32361
B	?	-	GLU	deletion	UNP P32361
B	?	-	HIS	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	ARG	deletion	UNP P32361
B	?	-	HIS	deletion	UNP P32361
B	?	-	THR	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	ASP	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	PHE	deletion	UNP P32361
B	?	-	TYR	deletion	UNP P32361
B	?	-	ASP	deletion	UNP P32361
B	?	-	PRO	deletion	UNP P32361
B	?	-	PHE	deletion	UNP P32361

- Molecule 2 is 5-AMINO-3-{{4-(AMINOSULFONYL)PHENYL}AMINO}-N-(2,6-DIFLUOROPHENYL)-1H-1,2,4-TRIAZOLE-1-CARBOTHIOAMIDE (CCD ID: DKI) (formula: $C_{15}H_{13}F_2N_7O_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			28	15	2	7	2	2		
2	B	1	Total	C	F	N	O	S	0	0
			28	15	2	7	2	2		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	125.55Å 125.55Å 174.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.26 – 3.33 51.26 – 3.33	Depositor EDS
% Data completeness (in resolution range)	98.3 (51.26-3.33) 98.2 (51.26-3.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.263 , 0.284 0.255 , 0.283	Depositor DCC
R_{free} test set	1181 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6348	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DKI, SEP, TPO

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	0.49	2/3181 (0.1%)	1.26	15/4309 (0.3%)
1	B	0.50	0/3181	0.78	3/4309 (0.1%)
All	All	0.50	2/6362 (0.0%)	1.05	18/8618 (0.2%)

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	2
1	B	1	2
All	All	1	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1106	ASP	CA-C	6.94	1.61	1.53
1	A	1106	ASP	CA-CB	5.64	1.60	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	862	GLU	CA-C-N	34.36	168.12	122.42
1	A	862	GLU	C-N-CA	34.36	168.12	122.42
1	A	897	LEU	N-CA-CB	-20.53	81.08	110.44
1	A	895	ARG	N-CA-CB	-19.76	80.99	110.04
1	A	863	GLU	N-CA-CB	18.29	139.28	110.21
1	A	896	ARG	CB-CA-C	-16.41	84.88	110.14
1	A	843	ARG	N-CA-CB	16.00	137.71	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	894	LYS	N-CA-CB	15.10	136.01	110.49
1	B	893	THR	CB-CA-C	13.62	137.52	110.42
1	A	842	PHE	N-CA-C	13.20	147.96	111.00
1	A	863	GLU	N-CA-C	-11.51	89.88	108.41
1	A	862	GLU	N-CA-C	-10.89	94.52	110.42
1	A	896	ARG	N-CA-C	-9.78	92.02	108.26
1	A	842	PHE	CB-CA-C	-6.31	98.11	110.10
1	A	895	ARG	N-CA-C	6.29	118.91	110.35
1	A	897	LEU	N-CA-C	6.29	118.65	110.53
1	B	894	LYS	N-CA-C	-6.08	97.85	110.80
1	A	1106	ASP	N-CA-C	5.11	117.25	107.75

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	893	THR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1003	ASP	Peptide
1	A	1076	VAL	Peptide
1	B	1003	ASP	Peptide
1	B	1076	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3146	0	3001	72	1
1	B	3146	0	3002	52	0
2	A	28	0	13	3	0
2	B	28	0	13	4	0
All	All	6348	0	6029	124	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (124) 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:842:PHE:CE2	1:A:897:LEU:HD13	1.34	1.56
1:A:842:PHE:CE2	1:A:897:LEU:CD1	1.85	1.56
1:A:842:PHE:CD2	1:A:897:LEU:CD1	2.14	1.31
1:A:842:PHE:CD2	1:A:897:LEU:HD12	1.66	1.29
1:A:843:ARG:H	1:A:896:ARG:HA	1.05	1.14
1:A:842:PHE:CZ	1:A:897:LEU:HD13	1.96	1.00
1:A:842:PHE:HE2	1:A:897:LEU:HD13	1.28	0.94
1:A:843:ARG:N	1:A:896:ARG:HA	1.82	0.93
1:A:843:ARG:H	1:A:896:ARG:CA	1.85	0.88
1:A:893:THR:HA	1:A:894:LYS:CB	2.04	0.86
1:A:1076:VAL:HG23	1:A:1077:PRO:HD2	1.59	0.82
1:B:1076:VAL:HG23	1:B:1077:PRO:HD2	1.62	0.81
1:A:685:SER:HA	1:B:682:TYR:CZ	2.16	0.79
1:A:1103:LEU:O	1:A:1106:ASP:HB2	1.82	0.79
1:B:812:THR:HG21	1:B:821:ASN:O	1.86	0.76
1:A:842:PHE:CD2	1:A:897:LEU:HD11	2.20	0.76
2:A:1:DKI:SAE	2:A:1:DKI:FAG	2.34	0.75
1:A:842:PHE:CZ	1:A:897:LEU:CD1	2.64	0.74
1:A:842:PHE:CG	1:A:897:LEU:HD12	2.22	0.73
1:A:785:VAL:HG21	1:A:906:MET:HE2	1.70	0.73
1:B:785:VAL:HG21	1:B:906:MET:HE2	1.72	0.71
1:B:865:ASN:HB3	1:B:868:GLN:HB2	1.72	0.71
1:A:861:LEU:O	1:A:862:GLU:C	2.34	0.71
1:A:812:THR:HG21	1:A:821:ASN:O	1.90	0.70
2:B:1:DKI:NAP	2:B:1:DKI:HAL	2.07	0.70
1:A:842:PHE:CE2	1:A:897:LEU:HD11	2.17	0.69
1:B:1081:TYR:CZ	1:B:1085:THR:HG21	2.28	0.68
2:A:1:DKI:NAP	2:A:1:DKI:HAL	2.08	0.67
1:A:925:TYR:OH	1:B:917:GLY:HA3	1.95	0.65
1:A:1081:TYR:CZ	1:A:1085:THR:HG21	2.31	0.65
1:A:673:LEU:HD21	1:A:744:ALA:HB2	1.79	0.65
1:B:805:VAL:HG22	1:B:824:ILE:HD13	1.79	0.64
1:B:673:LEU:HD21	1:B:744:ALA:HB2	1.80	0.63
1:B:811:PHE:CD1	1:B:823:ARG:HG2	2.33	0.63
1:B:868:GLN:O	1:B:893:THR:C	2.41	0.62
1:A:1106:ASP:C	1:A:1110:ARG:HG2	2.24	0.62
1:A:811:PHE:CD1	1:A:823:ARG:HG2	2.35	0.62
1:A:805:VAL:HG22	1:A:824:ILE:HD13	1.81	0.62
1:A:842:PHE:CE2	1:A:897:LEU:HD12	1.87	0.61
1:B:842:PHE:HD2	1:B:844:TPO:HG22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:842:PHE:CD2	1:B:844:TPO:HG22	2.36	0.61
1:A:842:PHE:CD2	1:A:844:TPO:HG22	2.36	0.60
1:A:857:ALA:HB3	1:A:901:ILE:CD1	2.31	0.60
1:A:842:PHE:HD2	1:A:844:TPO:HG22	1.67	0.59
1:B:1103:LEU:O	1:B:1106:ASP:HB2	2.01	0.59
1:B:857:ALA:HB3	1:B:901:ILE:CD1	2.33	0.58
1:A:843:ARG:N	1:A:896:ARG:CA	2.57	0.58
1:A:1106:ASP:O	1:A:1110:ARG:N	2.31	0.58
1:A:842:PHE:HE2	1:A:897:LEU:CD1	1.93	0.57
1:A:1100:LYS:O	1:A:1104:SER:HB3	2.05	0.56
1:A:925:TYR:HH	1:B:917:GLY:HA3	1.70	0.56
1:A:807:THR:HG22	1:A:822:LEU:CD2	2.36	0.55
1:A:997:LEU:HD21	1:A:1012:PHE:CE1	2.42	0.55
1:A:691:GLN:HG3	1:A:747:LEU:HD11	1.89	0.55
1:B:807:THR:HG22	1:B:822:LEU:CD2	2.37	0.55
1:A:685:SER:HA	1:B:682:TYR:CE2	2.42	0.54
1:B:691:GLN:HG3	1:B:747:LEU:HD11	1.89	0.54
1:B:680:LEU:HD22	2:B:1:DKI:CAK	2.39	0.53
1:B:997:LEU:HD21	1:B:1012:PHE:CE1	2.44	0.52
1:A:794:ILE:HD12	1:A:842:PHE:HE1	1.75	0.52
1:A:1076:VAL:HG23	1:A:1077:PRO:CD	2.34	0.52
1:A:843:ARG:O	1:A:844:TPO:C	2.58	0.52
1:A:807:THR:HG22	1:A:822:LEU:HD23	1.92	0.51
1:A:1003:ASP:CB	1:A:1004:PRO:HD3	2.41	0.51
1:B:843:ARG:O	1:B:844:TPO:C	2.58	0.51
1:B:1100:LYS:O	1:B:1104:SER:HB3	2.10	0.51
2:A:1:DKI:SAE	2:A:1:DKI:NAA	2.79	0.51
1:B:1076:VAL:HG23	1:B:1077:PRO:CD	2.35	0.51
1:B:794:ILE:HD12	1:B:842:PHE:HE1	1.76	0.50
1:B:857:ALA:HB3	1:B:901:ILE:HD12	1.94	0.50
1:B:835:LEU:HD13	1:B:840:SEP:HA	1.95	0.49
1:B:1003:ASP:CB	1:B:1004:PRO:HD3	2.42	0.49
1:A:774:PRO:O	1:A:778:LEU:HD13	2.12	0.49
1:A:1103:LEU:HB3	1:A:1106:ASP:OD2	2.13	0.49
1:A:1103:LEU:HD22	1:A:1106:ASP:OD2	2.12	0.48
1:A:835:LEU:HD13	1:A:840:SEP:HA	1.96	0.48
1:A:841:SEP:HA	1:A:897:LEU:O	2.12	0.48
1:B:1106:ASP:C	1:B:1110:ARG:HG2	2.38	0.48
1:A:989:PHE:O	1:A:993:VAL:HG23	2.13	0.48
1:A:833:LYS:NZ	1:A:844:TPO:HG21	2.28	0.48
1:B:807:THR:HG22	1:B:822:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:HIS:O	1:B:796:ARG:HB2	2.14	0.47
1:A:857:ALA:HB3	1:A:901:ILE:HD12	1.96	0.47
1:B:833:LYS:NZ	1:B:844:TPO:HG21	2.30	0.47
1:B:812:THR:CG2	1:B:821:ASN:O	2.60	0.47
1:B:989:PHE:O	1:B:993:VAL:HG23	2.15	0.47
1:A:1012:PHE:HA	1:A:1098:ILE:HD13	1.96	0.46
1:A:857:ALA:CB	1:A:901:ILE:HD12	2.46	0.46
2:B:1:DKI:SAE	2:B:1:DKI:NAA	2.88	0.46
1:B:750:LEU:HD23	1:B:750:LEU:N	2.31	0.45
2:B:1:DKI:NAP	2:B:1:DKI:CAL	2.73	0.45
1:B:1012:PHE:HA	1:B:1098:ILE:HD13	1.98	0.45
1:A:751:ASN:HA	1:A:804:LEU:HA	1.99	0.45
1:B:857:ALA:CB	1:B:901:ILE:HD12	2.47	0.45
1:A:1106:ASP:HB3	1:A:1109:LEU:HB2	1.99	0.45
1:B:860:LEU:CD1	1:B:901:ILE:HD11	2.46	0.45
1:B:725:HIS:CD2	1:B:727:ASN:H	2.35	0.44
1:B:751:ASN:HA	1:B:804:LEU:HA	1.99	0.44
1:B:866:ASN:C	1:B:868:GLN:H	2.25	0.44
1:A:812:THR:CG2	1:A:821:ASN:O	2.63	0.44
1:A:1099:VAL:HG13	1:A:1103:LEU:HB2	2.00	0.44
1:A:750:LEU:N	1:A:750:LEU:HD23	2.32	0.44
1:A:925:TYR:OH	1:B:757:GLU:HG2	2.18	0.44
1:B:1106:ASP:O	1:B:1110:ARG:N	2.46	0.43
1:A:1003:ASP:CB	1:A:1004:PRO:CD	2.97	0.43
1:A:725:HIS:CD2	1:A:727:ASN:H	2.37	0.43
1:B:774:PRO:O	1:B:778:LEU:HD13	2.18	0.43
1:B:1003:ASP:CB	1:B:1004:PRO:CD	2.97	0.42
1:A:795:HIS:O	1:A:796:ARG:HB2	2.20	0.41
1:A:868:GLN:HA	1:A:868:GLN:HE21	1.85	0.41
1:B:1103:LEU:HD22	1:B:1106:ASP:OD2	2.20	0.41
1:A:842:PHE:N	1:A:896:ARG:CB	2.84	0.41
1:B:773:ASN:HD22	1:B:774:PRO:HD2	1.85	0.41
1:A:729:ILE:CD1	1:A:746:GLU:HB3	2.51	0.41
1:A:773:ASN:HD22	1:A:774:PRO:HD2	1.85	0.41
1:A:867:LEU:H	1:A:867:LEU:HG	1.73	0.41
1:A:893:THR:CA	1:A:894:LYS:CB	2.83	0.41
1:A:944:LEU:HD13	1:A:949:LEU:HB3	2.02	0.41
1:A:833:LYS:HZ3	1:A:844:TPO:HG21	1.85	0.41
1:B:936:PHE:CD1	1:B:961:ILE:HD11	2.56	0.41
1:B:944:LEU:HD13	1:B:949:LEU:HB3	2.02	0.40
1:A:740:PHE:CZ	1:B:705:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:VAL:O	1:B:1078:ASP:N	2.54	0.40
1:B:1099:VAL:HG13	1:B:1103:LEU:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:ASN:ND2	1:A:996:ARG:NH2[6_555]	2.00	0.20

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	399/434 (92%)	371 (93%)	22 (6%)	6 (2%)	8	33
1	B	399/434 (92%)	370 (93%)	24 (6%)	5 (1%)	9	35
All	All	798/868 (92%)	741 (93%)	46 (6%)	11 (1%)	9	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	843	ARG
1	A	868	GLN
1	A	1076	VAL
1	A	1077	PRO
1	B	893	THR
1	B	1076	VAL
1	B	1077	PRO
1	A	894	LYS
1	B	894	LYS
1	B	1004	PRO
1	A	1004	PRO

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	323/395 (82%)	311 (96%)	12 (4%)	30	57
1	B	323/395 (82%)	313 (97%)	10 (3%)	35	61
All	All	646/790 (82%)	624 (97%)	22 (3%)	32	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	746	GLU
1	A	777	LEU
1	A	796	ARG
1	A	856	ARG
1	A	867	LEU
1	A	868	GLN
1	A	897	LEU
1	A	942	LYS
1	A	1053	ARG
1	A	1063	MET
1	A	1087	ARG
1	A	1109	LEU
1	B	746	GLU
1	B	777	LEU
1	B	796	ARG
1	B	823	ARG
1	B	856	ARG
1	B	942	LYS
1	B	1053	ARG
1	B	1063	MET
1	B	1087	ARG
1	B	1109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	773	ASN
1	A	787	HIS
1	A	816	GLN
1	A	868	GLN
1	A	1057	ASN
1	A	1060	HIS
1	A	1090	ASN
1	B	773	ASN
1	B	787	HIS
1	B	815	GLN
1	B	816	GLN
1	B	1060	HIS
1	B	1090	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	SEP	A	840	1	8,9,10	1.71	1 (12%)	7,12,14	1.67	1 (14%)
1	SEP	A	841	1	8,9,10	1.66	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	B	841	1	8,9,10	1.73	2 (25%)	7,12,14	1.56	1 (14%)
1	TPO	B	844	1	8,10,11	0.88	0	10,14,16	1.01	0
1	SEP	B	840	1	8,9,10	1.79	2 (25%)	7,12,14	1.60	1 (14%)
1	TPO	A	844	1	8,10,11	0.97	1 (12%)	10,14,16	0.95	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	SEP	A	840	1	-	1/6/8/10	-
1	SEP	A	841	1	-	4/6/8/10	-
1	SEP	B	841	1	-	4/6/8/10	-
1	TPO	B	844	1	-	4/9/11/13	-
1	SEP	B	840	1	-	0/6/8/10	-
1	TPO	A	844	1	-	4/9/11/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	840	SEP	P-O1P	3.86	1.62	1.50
1	B	841	SEP	P-O1P	3.78	1.62	1.50
1	A	840	SEP	P-O1P	3.74	1.62	1.50
1	A	841	SEP	P-O1P	3.67	1.61	1.50
1	B	840	SEP	P-O3P	2.12	1.62	1.54
1	A	844	TPO	P-OG1	2.07	1.63	1.59
1	B	841	SEP	P-O3P	2.01	1.62	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	840	SEP	OG-CB-CA	3.99	112.02	108.14
1	B	840	SEP	OG-CB-CA	3.82	111.87	108.14
1	B	841	SEP	OG-CB-CA	3.35	111.40	108.14
1	A	841	SEP	OG-CB-CA	2.72	110.79	108.14

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	841	SEP	N-CA-CB-OG
1	A	841	SEP	C-CA-CB-OG
1	A	844	TPO	N-CA-CB-CG2
1	A	844	TPO	N-CA-CB-OG1
1	A	844	TPO	C-CA-CB-CG2
1	B	841	SEP	N-CA-CB-OG
1	B	841	SEP	C-CA-CB-OG
1	B	844	TPO	N-CA-CB-CG2
1	B	844	TPO	N-CA-CB-OG1
1	B	844	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
1	A	841	SEP	CB-OG-P-O2P
1	A	841	SEP	CA-CB-OG-P
1	B	841	SEP	CA-CB-OG-P
1	A	840	SEP	CB-OG-P-O2P
1	B	841	SEP	CB-OG-P-O2P
1	A	844	TPO	O-C-CA-CB
1	B	844	TPO	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	840	SEP	1	0
1	A	841	SEP	1	0
1	B	844	TPO	4	0
1	B	840	SEP	1	0
1	A	844	TPO	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	DKI	A	1	-	30,30,30	3.37	8 (26%)	40,44,44	2.25	9 (22%)
2	DKI	B	1	-	30,30,30	3.13	8 (26%)	40,44,44	1.94	8 (20%)

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	DKI	A	1	-	-	4/17/18/18	0/3/3/3
2	DKI	B	1	-	-	4/17/18/18	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	DKI	CAY-SBB	-11.03	1.60	1.77
2	B	1	DKI	CAY-SBB	-10.50	1.61	1.77
2	A	1	DKI	CAS-SAE	-7.38	1.55	1.67
2	B	1	DKI	CAZ-CAU	6.99	1.48	1.38
2	A	1	DKI	CAZ-CAV	6.94	1.48	1.38
2	A	1	DKI	CAZ-CAU	6.85	1.48	1.38
2	B	1	DKI	CAZ-CAV	6.15	1.47	1.38
2	B	1	DKI	CAS-SAE	-5.96	1.58	1.67
2	A	1	DKI	CAS-NBA	-5.38	1.36	1.40
2	B	1	DKI	CAZ-NAQ	-5.13	1.34	1.43
2	A	1	DKI	CAZ-NAQ	-4.07	1.36	1.43
2	B	1	DKI	CAS-NBA	-3.80	1.37	1.40
2	B	1	DKI	CAT-NBA	-2.83	1.32	1.37
2	A	1	DKI	CAT-NBA	-2.81	1.32	1.37
2	A	1	DKI	CAW-NAR	-2.23	1.37	1.41
2	B	1	DKI	CAW-NAR	-2.15	1.37	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	DKI	OAD-SBB-OAC	-6.50	108.80	118.80
2	B	1	DKI	OAD-SBB-OAC	-6.11	109.40	118.80
2	A	1	DKI	CAU-CAZ-NAQ	-5.48	115.21	122.12
2	A	1	DKI	CAZ-NAQ-CAS	5.26	130.68	123.03
2	B	1	DKI	CAZ-NAQ-CAS	-4.93	115.87	123.03
2	A	1	DKI	CAV-CAZ-NAQ	4.65	127.98	122.12
2	B	1	DKI	CAV-CAZ-NAQ	-3.70	117.45	122.12
2	A	1	DKI	FAG-CAV-CAZ	3.53	121.30	117.64
2	A	1	DKI	OAC-SBB-CAY	3.50	111.31	107.35
2	B	1	DKI	FAF-CAU-CAZ	3.10	120.86	117.64
2	B	1	DKI	CAI-CAU-CAZ	-2.78	118.84	122.83
2	A	1	DKI	OAD-SBB-NAB	2.74	111.31	107.35
2	B	1	DKI	OAD-SBB-CAY	2.70	110.41	107.35
2	B	1	DKI	CAJ-CAV-CAZ	-2.40	119.39	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	DKI	SAE-CAS-NAQ	2.21	128.10	123.42
2	A	1	DKI	CAJ-CAV-CAZ	-2.21	119.67	122.83
2	A	1	DKI	CAI-CAU-CAZ	-2.19	119.69	122.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

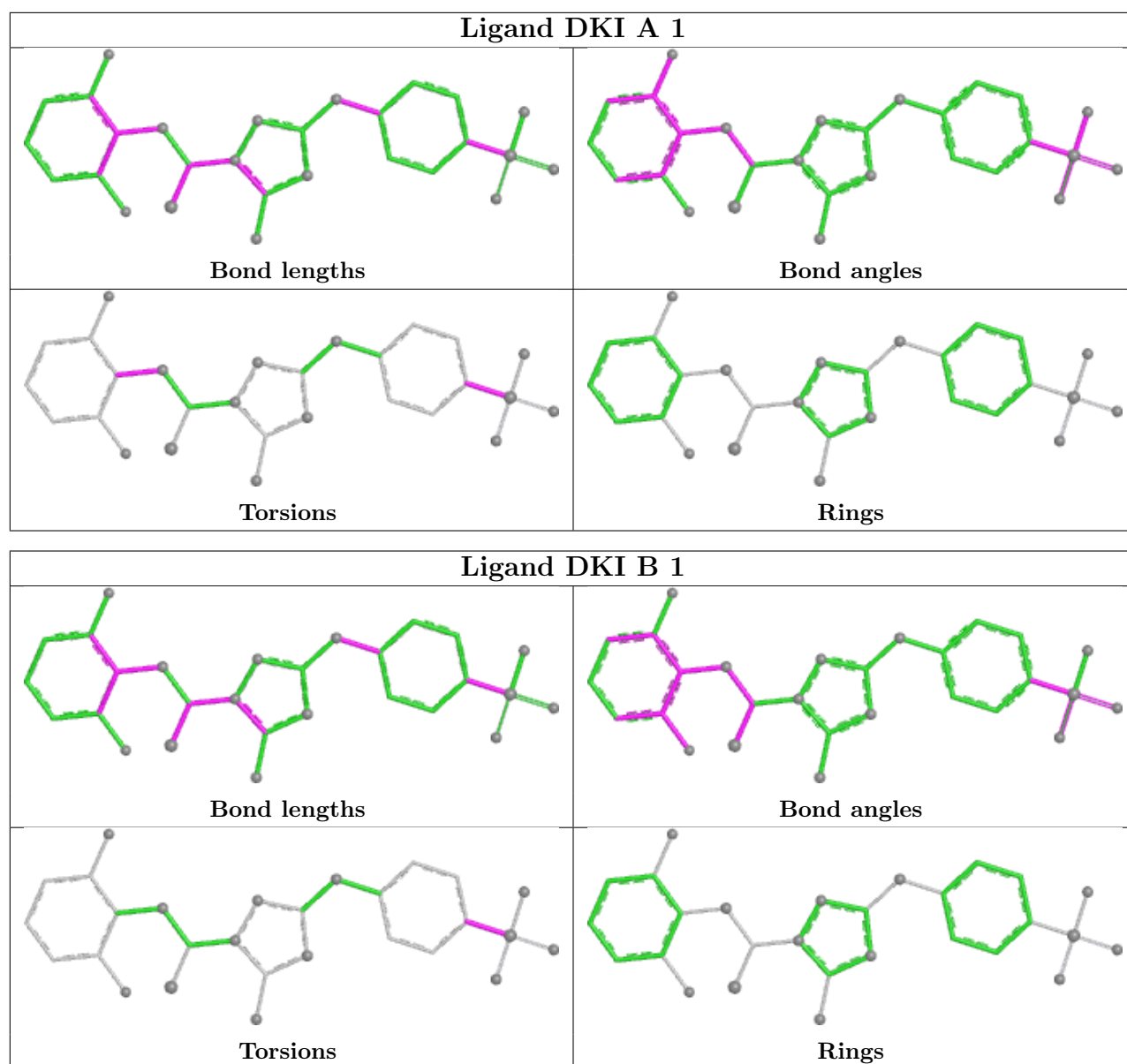
Mol	Chain	Res	Type	Atoms
2	A	1	DKI	CAU-CAZ-NAQ-CAS
2	A	1	DKI	CAV-CAZ-NAQ-CAS
2	B	1	DKI	CAM-CAY-SBB-NAB
2	B	1	DKI	CAN-CAY-SBB-OAC
2	B	1	DKI	CAM-CAY-SBB-OAC
2	B	1	DKI	CAN-CAY-SBB-NAB
2	A	1	DKI	CAN-CAY-SBB-OAD
2	A	1	DKI	CAM-CAY-SBB-OAD

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	DKI	3	0
2	B	1	DKI	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/434 (93%)	0.92	65 (16%) 4 5	48, 69, 101, 159	0
1	B	404/434 (93%)	0.64	51 (12%) 8 7	35, 54, 82, 103	0
All	All	808/868 (93%)	0.78	116 (14%) 6 6	35, 62, 96, 159	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	893	THR	6.6
1	A	686	GLY	6.3
1	A	1106	ASP	6.1
1	A	818	GLY	5.8
1	A	862	GLU	5.2
1	A	819	ALA	5.2
1	A	817	THR	5.2
1	B	809	SER	4.8
1	A	665	ASN	4.7
1	A	707	ASP	4.6
1	B	817	THR	4.6
1	B	818	GLY	4.5
1	A	666	PHE	4.5
1	B	813	ALA	4.4
1	A	1030	ASP	4.4
1	A	865	ASN	4.4
1	B	665	ASN	4.3
1	A	1049	MET	4.2
1	B	1038	GLU	4.1
1	A	843	ARG	4.1
1	B	1106	ASP	4.1
1	B	819	ALA	4.0
1	A	1042	LYS	4.0
1	B	808	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	709	CYS	3.9
1	A	866	ASN	3.8
1	B	1003	ASP	3.8
1	A	709	CYS	3.7
1	A	685	SER	3.7
1	B	684	SER	3.7
1	B	669	SER	3.6
1	A	1107	GLN	3.6
1	B	1040	TYR	3.6
1	A	815	GLN	3.5
1	B	816	GLN	3.5
1	A	894	LYS	3.5
1	A	813	ALA	3.5
1	A	1105	ASP	3.5
1	B	814	ASP	3.5
1	B	867	LEU	3.4
1	A	714	MET	3.4
1	B	707	ASP	3.4
1	A	821	ASN	3.2
1	A	864	SER	3.1
1	A	668	GLN	3.1
1	A	816	GLN	3.1
1	A	925	TYR	3.1
1	B	811	PHE	3.0
1	A	1039	ARG	3.0
1	A	838	GLY	3.0
1	B	682	TYR	3.0
1	A	1101	GLU	2.9
1	B	1105	ASP	2.9
1	A	933	ARG	2.9
1	A	943	CYS	2.9
1	B	894	LYS	2.8
1	A	1003	ASP	2.8
1	B	810	ARG	2.8
1	A	863	GLU	2.8
1	A	810	ARG	2.7
1	A	1104	SER	2.7
1	B	812	THR	2.7
1	A	1035	ASP	2.7
1	A	852	THR	2.7
1	B	703	ARG	2.7
1	B	1030	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	705	LEU	2.7
1	A	706	ILE	2.6
1	A	711	ILE	2.6
1	A	1040	TYR	2.6
1	A	867	LEU	2.6
1	B	724	ASP	2.6
1	B	708	PHE	2.6
1	A	836	ASP	2.6
1	A	839	GLN	2.6
1	B	868	GLN	2.6
1	B	866	ASN	2.6
1	B	666	PHE	2.6
1	A	1038	GLU	2.6
1	A	687	THR	2.6
1	A	677	GLU	2.5
1	B	1107	GLN	2.5
1	A	895	ARG	2.5
1	B	705	LEU	2.5
1	A	1034	MET	2.5
1	A	738	ASP	2.5
1	A	667	GLU	2.4
1	A	811	PHE	2.4
1	B	1035	ASP	2.4
1	A	820	GLU	2.4
1	A	893	THR	2.4
1	B	852	THR	2.3
1	B	1067	GLU	2.3
1	A	669	SER	2.2
1	A	758	SER	2.2
1	B	668	GLN	2.2
1	B	863	GLU	2.2
1	B	1049	MET	2.2
1	B	685	SER	2.2
1	A	868	GLN	2.2
1	A	1057	ASN	2.2
1	B	807	THR	2.2
1	A	937	SER	2.2
1	B	815	GLN	2.2
1	B	696	GLY	2.2
1	A	741	LEU	2.1
1	B	1042	LYS	2.1
1	B	896	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1041	ARG	2.1
1	A	1060	HIS	2.1
1	B	706	ILE	2.1
1	B	687	THR	2.1
1	B	740	PHE	2.1
1	A	720	THR	2.0
1	A	708	PHE	2.0
1	B	674	VAL	2.0

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, 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(Å ²)	Q<0.9
1	SEP	A	840	10/11	0.74	0.22	81,88,93,97	0
1	TPO	A	844	11/12	0.77	0.19	82,87,92,94	0
1	SEP	A	841	10/11	0.78	0.18	87,91,103,106	0
1	TPO	B	844	11/12	0.81	0.18	61,62,64,65	0
1	SEP	B	841	10/11	0.87	0.18	59,63,69,70	0
1	SEP	B	840	10/11	0.88	0.17	56,60,64,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

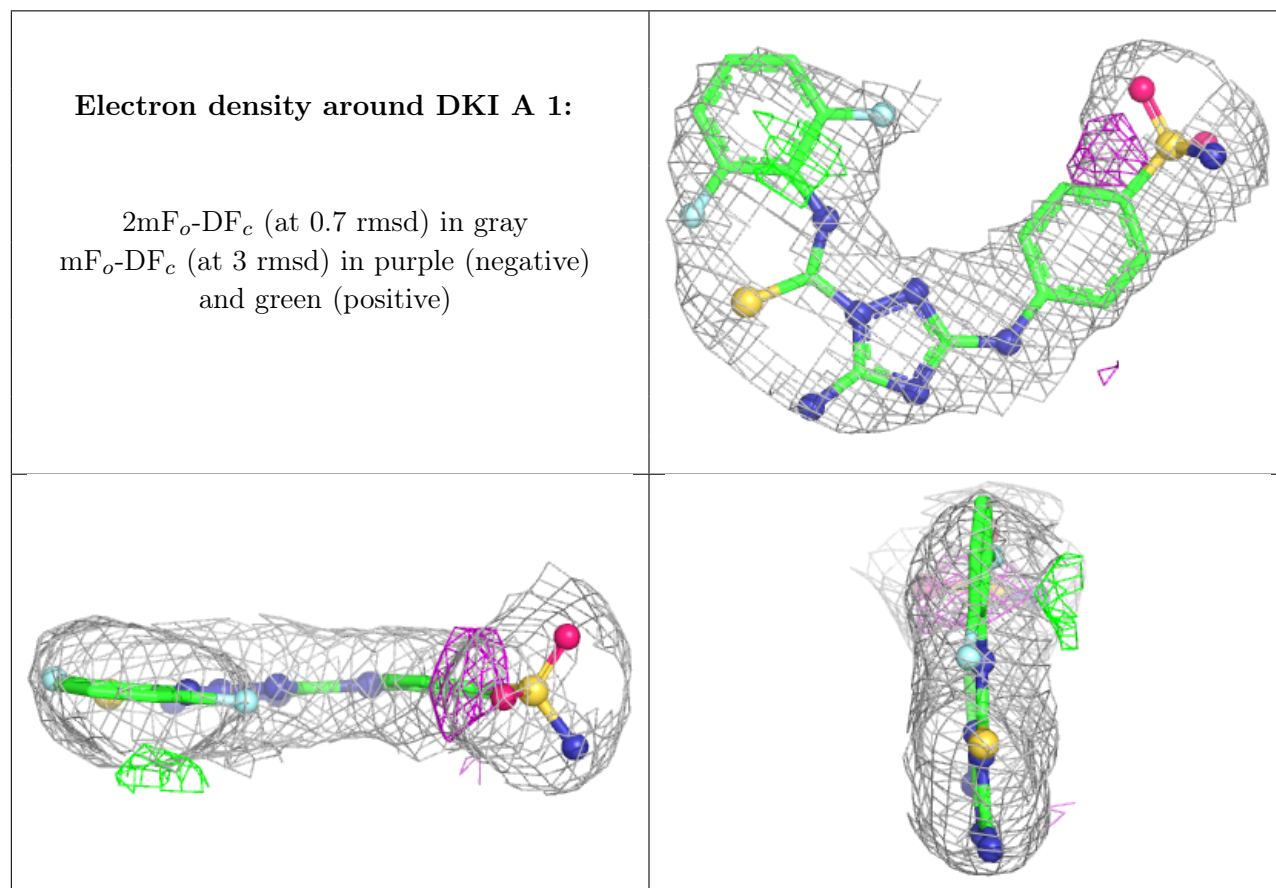
6.4 Ligands [i](#)

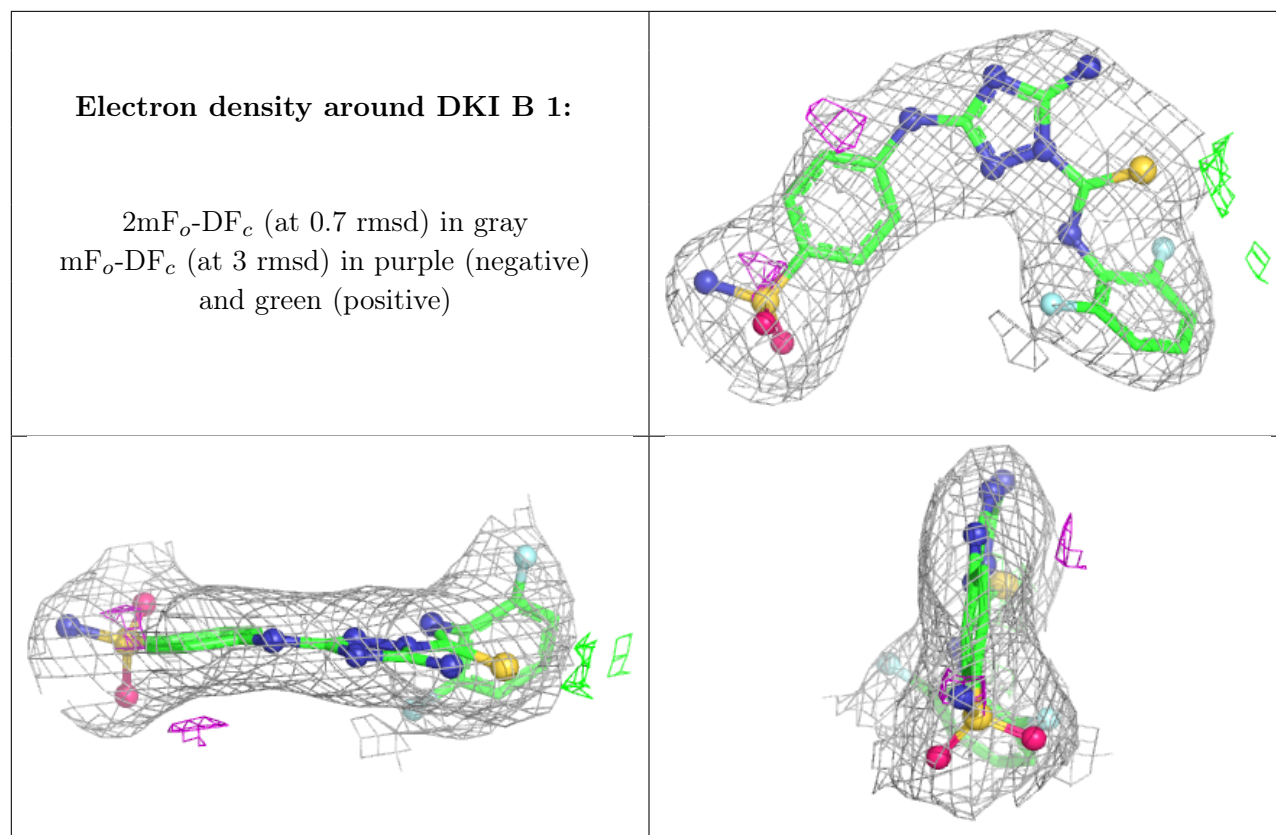
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DKI	A	1	28/28	0.92	0.11	53,56,66,67	0
2	DKI	B	1	28/28	0.96	0.08	42,43,48,48	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.