Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 09:25 PM UTC

PDB ID	:	6RSH / pdb_00006rsh
Title	:	Structure based optimization of JAK1-ATP binding pocket Inhibitors in the aminopyrazole class
Authors	:	Brown, D.G.; Lupardus, P.J.
Deposited on	:	2019-05-21
Resolution	:	1.71 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:

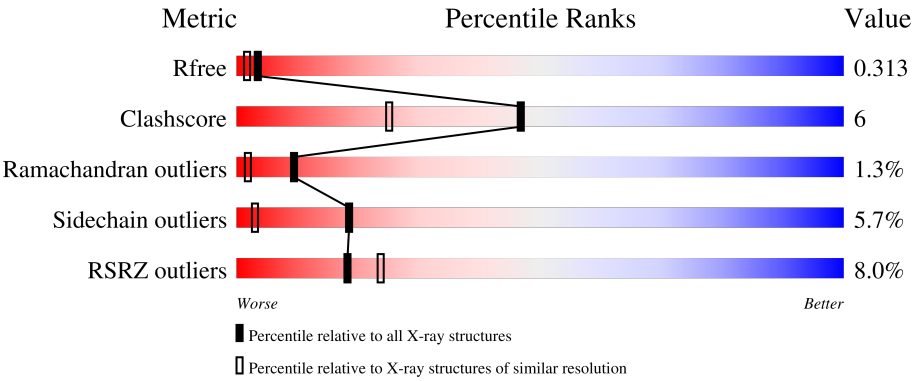
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 1.71 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	302	7% 73% 20% • 5%
1	B	302	8% 76% 13% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5030 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.

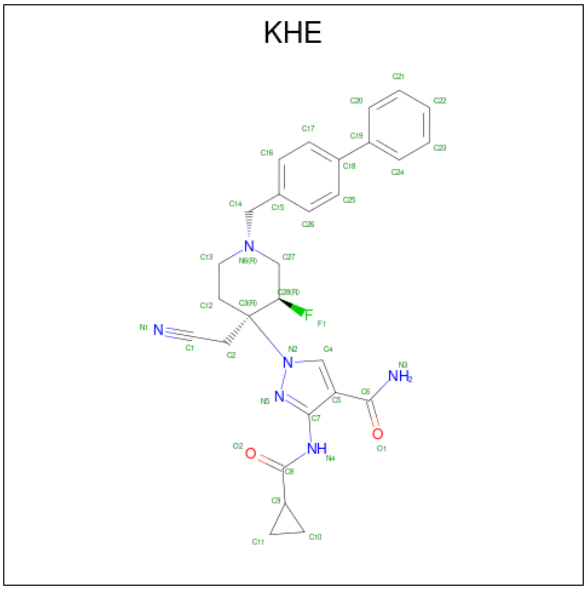
- Molecule 1 is a protein called Tyrosine-protein kinase JAK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	1	0
			2331	1482	395	437	2	15			
1	B	281	Total	C	N	O	P	S	0	0	0
			2291	1461	388	425	2	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	-	expression tag	UNP P23458
B	853	GLY	-	expression tag	UNP P23458

- Molecule 2 is 1-[(3 {R},4 {R})-4-(cyanomethyl)-3-fluoranyl-1-[(4-phenylphenyl)methyl]piperidin-4-yl]-3-(cyclopropylcarbonylamino)pyrazole-4-carboxamide (CCD ID: KHE) (formula: $C_{28}H_{29}FN_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	28	1	6	2		
2	B	1	Total	C	F	N	O	0	0
			37	28	1	6	2		

- Molecule 3 is water.

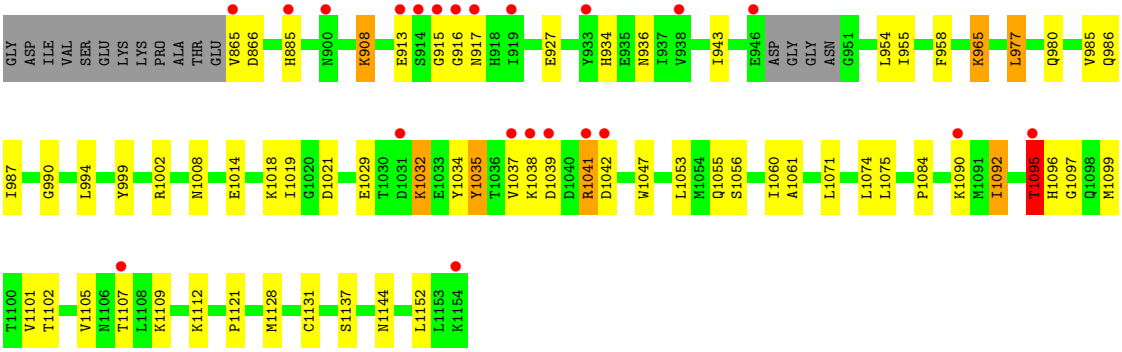
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	170	Total	O	0	0
			170	170		

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.

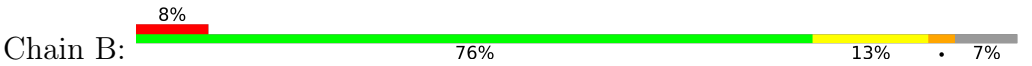
• Molecule 1: Tyrosine-protein kinase JAK1

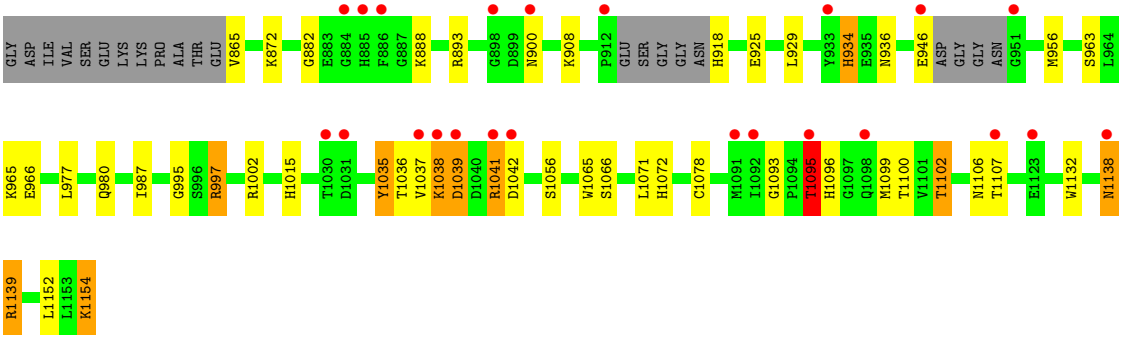
Chain A:



• Molecule 1: Tyrosine-protein kinase JAK1

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	43.01Å 89.18Å 174.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 1.71 48.76 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.76-1.71) 99.9 (48.76-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.269 , 0.311 0.273 , 0.313	Depositor DCC
R_{free} test set	3691 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 25.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5030	wwPDB-VP
Average B, all atoms (Å^2)	14.0	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 56.98 % 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 2.5284e-05. 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: KHE, PTR

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	1.35	17/2347 (0.7%)	1.47	5/3159 (0.2%)
1	B	1.34	7/2306 (0.3%)	1.45	6/3103 (0.2%)
All	All	1.34	24/4653 (0.5%)	1.46	11/6262 (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	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1071	LEU	C-O	10.22	1.35	1.24
1	A	958	PHE	C-O	-7.39	1.15	1.24
1	A	1071	LEU	C-O	7.25	1.32	1.24
1	B	956	MET	C-O	7.23	1.32	1.23
1	A	1060	ILE	C-O	6.83	1.32	1.24
1	A	986	GLN	C-O	6.74	1.32	1.24
1	A	908	LYS	C-O	6.73	1.32	1.24
1	A	977	LEU	C-O	6.28	1.31	1.24
1	A	1102	THR	C-O	6.07	1.31	1.24
1	A	1121	PRO	C-O	5.99	1.30	1.23
1	B	882	GLY	C-O	5.91	1.29	1.23
1	B	1102	THR	C-O	5.88	1.31	1.24
1	A	990	GLY	C-O	5.86	1.30	1.23
1	B	995	GLY	C-O	5.72	1.30	1.23
1	A	1074	LEU	C-O	5.57	1.30	1.24
1	A	955	ILE	C-O	5.51	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1018	LYS	C-O	5.45	1.30	1.23
1	B	934	HIS	CE1-NE2	5.27	1.37	1.32
1	A	1041	ARG	C-O	5.25	1.30	1.23
1	A	1021	ASP	C-O	5.22	1.30	1.23
1	A	1061	ALA	C-O	5.15	1.30	1.24
1	B	1072	HIS	C-O	5.13	1.29	1.24
1	A	985	VAL	C-O	5.04	1.29	1.24
1	A	1008	ASN	N-CA	5.03	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1095	THR	CB-CA-C	6.96	124.28	110.42
1	B	1039	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	1066	SER	CA-C-O	-6.73	113.36	120.63
1	A	1019	ILE	CA-C-O	-6.03	113.66	120.95
1	A	1095	THR	CB-CA-C	5.81	121.99	110.42
1	B	1100	THR	CA-CB-OG1	-5.73	101.00	109.60
1	A	866	ASP	CB-CA-C	5.69	117.57	109.38
1	B	1138	ASN	CB-CA-C	5.47	121.30	110.42
1	B	987	ILE	CA-C-O	-5.25	115.60	121.17
1	A	1101	VAL	CA-C-O	-5.24	115.50	120.95
1	A	987	ILE	CA-C-O	-5.13	115.74	121.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	916	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2331	0	2315	26	0
1	B	2291	0	2286	30	0
2	A	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	37	0	0	0	0
3	A	164	0	0	6	0
3	B	170	0	0	7	0
All	All	5030	0	4601	53	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 (53) 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:1035:PTR:HE1	1:A:1037:VAL:HG22	1.53	0.90
1:A:934:HIS:HD2	1:A:936:ASN:H	1.27	0.82
1:B:977:LEU:HA	1:B:980:GLN:HE21	1.44	0.82
1:B:1035:PTR:HE1	1:B:1037:VAL:HG22	1.62	0.81
1:A:1097:GLY:HA3	1:B:1041:ARG:HD3	1.68	0.76
1:A:1053:LEU:O	1:B:1102:THR:HG21	1.85	0.75
1:A:977:LEU:HA	1:A:980:GLN:HE21	1.51	0.75
1:A:934:HIS:CD2	1:A:936:ASN:H	2.03	0.75
1:B:1015:HIS:ND1	3:B:1301:HOH:O	2.18	0.74
1:B:934:HIS:HD2	1:B:936:ASN:H	1.35	0.73
1:B:934:HIS:CD2	1:B:936:ASN:H	2.08	0.70
1:A:1035:PTR:CE1	1:A:1037:VAL:HG22	2.28	0.62
1:A:927:GLU:OE2	3:A:1301:HOH:O	2.16	0.61
1:A:915:GLY:O	1:A:917:ASN:HA	2.03	0.59
1:B:946:GLU:HA	1:B:946:GLU:OE1	2.04	0.56
1:B:1154:LYS:HA	1:B:1154:LYS:CE	2.38	0.53
1:A:1002:ARG:CZ	1:A:1037:VAL:HG21	2.38	0.53
1:A:934:HIS:HE1	3:A:1453:HOH:O	1.91	0.53
1:A:954:LEU:HD13	3:A:1395:HOH:O	2.08	0.52
1:B:1035:PTR:CE1	1:B:1037:VAL:HG22	2.37	0.52
1:B:1093:GLY:HA3	1:B:1096:HIS:CE1	2.44	0.52
1:B:934:HIS:HE1	3:B:1453:HOH:O	1.92	0.51
1:B:1036:THR:O	1:B:1038:LYS:HE2	2.11	0.51
1:B:997:ARG:HH11	1:B:997:ARG:HB3	1.77	0.49
1:B:1102:THR:HG23	3:B:1302:HOH:O	2.12	0.48
1:A:965:LYS:HD2	3:A:1384:HOH:O	2.11	0.48
1:B:1102:THR:O	3:B:1302:HOH:O	2.20	0.46
1:B:1106:ASN:HA	3:B:1303:HOH:O	2.16	0.45
1:A:908:LYS:HB3	1:A:954:LEU:HB3	1.98	0.45
1:B:1093:GLY:HA3	1:B:1096:HIS:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:LEU:HD12	1:A:1128:MET:CE	2.47	0.44
1:B:1065:TRP:CE3	1:B:1132:TRP:HA	2.53	0.44
1:B:997:ARG:HH11	1:B:997:ARG:CB	2.31	0.44
1:B:1154:LYS:HE3	3:B:1323:HOH:O	2.17	0.44
1:A:1105:VAL:O	1:A:1109:LYS:HG3	2.18	0.43
1:A:1047:TRP:CZ2	1:A:1084:PRO:HG2	2.53	0.43
1:A:943:ILE:HG22	3:A:1395:HOH:O	2.19	0.43
1:B:963:SER:OG	1:B:966:GLU:OE2	2.31	0.43
1:B:1002:ARG:CZ	1:B:1037:VAL:HG21	2.49	0.43
1:B:965:LYS:HD2	1:B:1078:CYS:HB3	2.00	0.42
1:B:918:HIS:N	3:B:1315:HOH:O	2.52	0.42
1:B:893:ARG:NE	1:B:900:ASN:ND2	2.68	0.42
1:B:1138:ASN:O	1:B:1139:ARG:O	2.38	0.42
1:A:1092:ILE:HG22	1:A:1107:THR:OG1	2.20	0.41
1:B:1099:MET:HE2	1:B:1099:MET:N	2.35	0.41
1:A:1075:LEU:HD12	1:A:1128:MET:HE1	2.01	0.41
1:A:1055:GLN:C	1:A:1056:SER:OG	2.62	0.41
1:A:954:LEU:CD1	3:A:1395:HOH:O	2.69	0.41
1:A:994:LEU:HG	1:A:999:TYR:HB2	2.02	0.41
1:A:1029:GLU:O	1:A:1032:LYS:HB2	2.21	0.40
1:B:908:LYS:NZ	1:B:925:GLU:OE2	2.38	0.40
1:A:1097:GLY:CA	1:B:1041:ARG:HD3	2.45	0.40
1:A:1128:MET:O	1:A:1131:CYS:HB2	2.21	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	281/302 (93%)	268 (95%)	9 (3%)	4 (1%)	9 2
1	B	273/302 (90%)	263 (96%)	7 (3%)	3 (1%)	11 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	554/604 (92%)	531 (96%)	16 (3%)	7 (1%)	9 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	913	GLU
1	B	1139	ARG
1	A	1095	THR
1	A	1096	HIS
1	A	1042	ASP
1	B	1042	ASP
1	B	1095	THR

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	256/267 (96%)	240 (94%)	16 (6%)	16 2
1	B	252/267 (94%)	239 (95%)	13 (5%)	21 3
All	All	508/534 (95%)	479 (94%)	29 (6%)	18 3

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	865	VAL
1	A	885	HIS
1	A	965	LYS
1	A	1014	GLU
1	A	1032	LYS
1	A	1038	LYS
1	A	1039	ASP
1	A	1041	ARG
1	A	1090	LYS
1	A	1092	ILE
1	A	1095	THR

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Mol	Chain	Res	Type
1	A	1099	MET
1	A	1112	LYS
1	A	1137	SER
1	A	1144	ASN
1	A	1152	LEU
1	B	865	VAL
1	B	872	LYS
1	B	888	LYS
1	B	929	LEU
1	B	997	ARG
1	B	1038	LYS
1	B	1039	ASP
1	B	1041	ARG
1	B	1056	SER
1	B	1095	THR
1	B	1107	THR
1	B	1152	LEU
1	B	1154	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	934	HIS
1	A	936	ASN
1	A	979	GLN
1	A	980	GLN
1	A	1098	GLN
1	A	1106	ASN
1	A	1135	GLN
1	A	1143	GLN
1	B	900	ASN
1	B	934	HIS
1	B	936	ASN
1	B	979	GLN
1	B	980	GLN
1	B	1096	HIS
1	B	1098	GLN
1	B	1138	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PTR	B	1034	1	15,16,17	0.94	0	17,22,24	0.90	0
1	PTR	A	1034	1	15,16,17	0.91	1 (6%)	17,22,24	0.87	0
1	PTR	B	1035	1	15,16,17	0.54	0	17,22,24	1.46	4 (23%)
1	PTR	A	1035	1	15,16,17	0.68	0	17,22,24	1.97	6 (35%)

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	PTR	B	1034	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1034	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1035	1	-	1/10/11/13	0/1/1/1
1	PTR	A	1035	1	-	0/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1034	PTR	P-OH	-2.90	1.54	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1035	PTR	OH-P-O1P	-4.68	93.88	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1035	PTR	O3P-P-OH	-3.63	94.58	105.32
1	A	1035	PTR	OH-CZ-CE1	-3.34	109.20	119.22
1	A	1035	PTR	OH-CZ-CE2	2.79	127.58	119.22
1	B	1035	PTR	O2P-P-OH	2.43	112.50	105.32
1	A	1035	PTR	O2P-P-OH	2.38	112.36	105.32
1	B	1035	PTR	OH-CZ-CE1	-2.13	112.83	119.22
1	A	1035	PTR	CE2-CZ-CE1	2.07	123.18	120.16
1	B	1035	PTR	OH-CZ-CE2	2.04	125.34	119.22
1	A	1035	PTR	CD2-CE2-CZ	-2.04	117.40	119.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1035	PTR	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1035	PTR	2	0
1	A	1035	PTR	2	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	KHE	A	1201	-	39,41,41	1.39	2 (5%)	45,59,59	1.17	5 (11%)
2	KHE	B	1201	-	39,41,41	0.80	2 (5%)	45,59,59	0.94	3 (6%)

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	KHE	A	1201	-	-	0/25/48/48	0/5/5/5
2	KHE	B	1201	-	-	0/25/48/48	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	KHE	C3-N2	-7.44	1.43	1.50
2	B	1201	KHE	C19-C18	-3.00	1.41	1.49
2	A	1201	KHE	C19-C18	-2.68	1.42	1.49
2	B	1201	KHE	C9-C8	-2.31	1.47	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	KHE	C4-N2-N5	-3.81	109.43	112.65
2	B	1201	KHE	C5-C7-N5	-3.05	109.51	113.81
2	A	1201	KHE	C2-C1-N1	-3.03	174.34	178.16
2	A	1201	KHE	C5-C7-N5	-2.84	109.81	113.81
2	B	1201	KHE	C4-N2-N5	-2.52	110.52	112.65
2	A	1201	KHE	C12-C3-N2	2.24	112.03	109.09
2	B	1201	KHE	C12-C3-N2	2.21	112.00	109.09
2	A	1201	KHE	C4-C5-C6	2.13	130.96	125.03

There are no chirality outliers.

There are no torsion outliers.

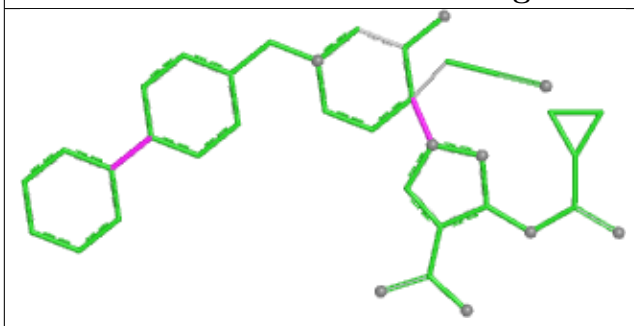
There are no ring outliers.

No monomer is involved in short contacts.

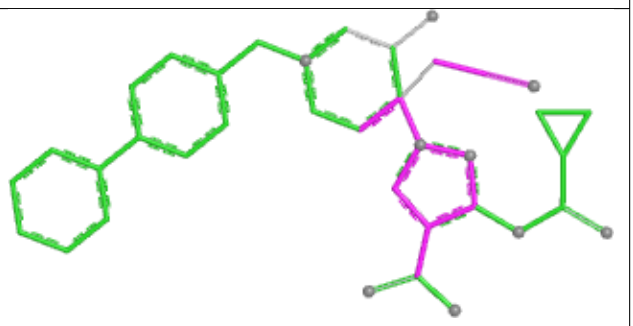
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

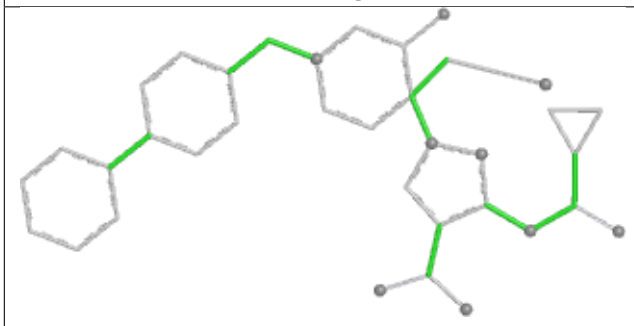
Ligand KHE A 1201



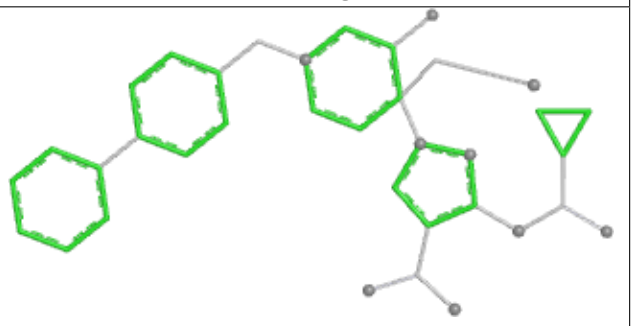
Bond lengths



Bond angles

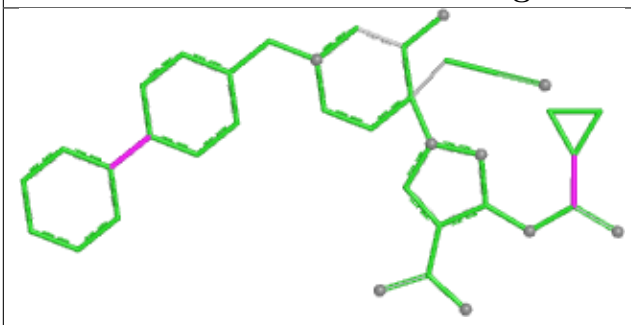


Torsions

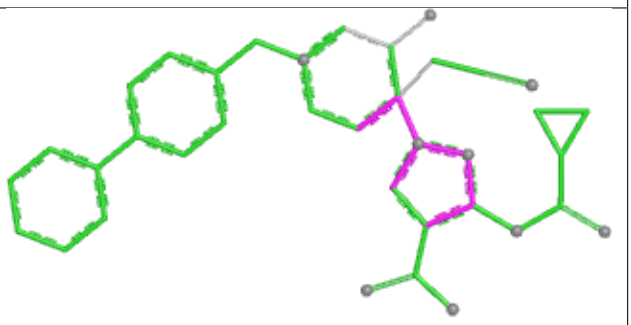


Rings

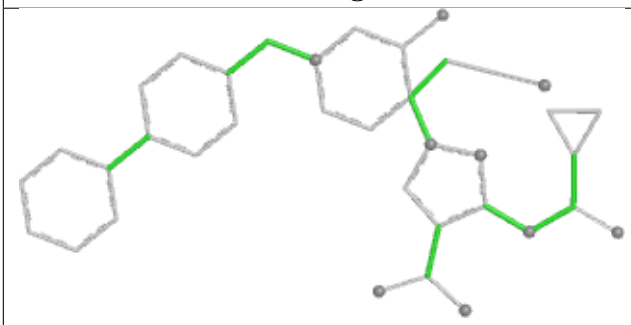
Ligand KHE B 1201



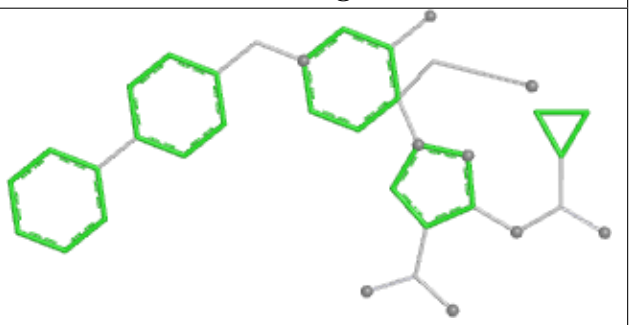
Bond lengths



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	284/302 (94%)	0.69	22 (7%)	19	25	6, 11, 28, 57	1 (0%)
1	B	279/302 (92%)	0.74	23 (8%)	17	23	5, 11, 26, 43	0
All	All	563/604 (93%)	0.72	45 (7%)	18	24	5, 11, 27, 57	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1095	THR	6.9
1	A	916	GLY	5.7
1	A	946	GLU	4.4
1	A	915	GLY	4.2
1	B	1031	ASP	4.0
1	B	1039	ASP	4.0
1	B	1095	THR	4.0
1	A	885	HIS	3.9
1	A	1031	ASP	3.9
1	A	1041	ARG	3.8
1	B	885	HIS	3.6
1	A	914	SER	3.5
1	A	865	VAL	3.5
1	B	1041	ARG	3.3
1	B	1098	GLN	3.3
1	B	886	PHE	3.2
1	B	900	ASN	3.2
1	A	917	ASN	3.1
1	B	933	TYR	3.1
1	A	933	TYR	3.0
1	B	1138	ASN	2.9
1	A	913	GLU	2.9
1	A	1037	VAL	2.9
1	B	951	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1030	THR	2.8
1	B	946	GLU	2.6
1	A	1090	LYS	2.6
1	B	1092	ILE	2.6
1	B	1107	THR	2.5
1	B	912	PRO	2.5
1	B	1037	VAL	2.4
1	B	1123	GLU	2.4
1	A	1042	ASP	2.3
1	B	884	GLY	2.3
1	A	938	VAL	2.3
1	B	1042	ASP	2.3
1	A	919	ILE	2.2
1	A	1107	THR	2.2
1	A	1154	LYS	2.2
1	B	898	GLY	2.2
1	A	1038	LYS	2.2
1	A	900	ASN	2.1
1	B	1091	MET	2.1
1	A	1039	ASP	2.1
1	B	1038	LYS	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, 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
1	PTR	B	1034	16/17	0.74	0.15	17,19,25,26	0
1	PTR	A	1035	16/17	0.83	0.12	13,23,32,32	0
1	PTR	A	1034	16/17	0.83	0.14	15,17,22,23	0
1	PTR	B	1035	16/17	0.83	0.13	15,25,31,31	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

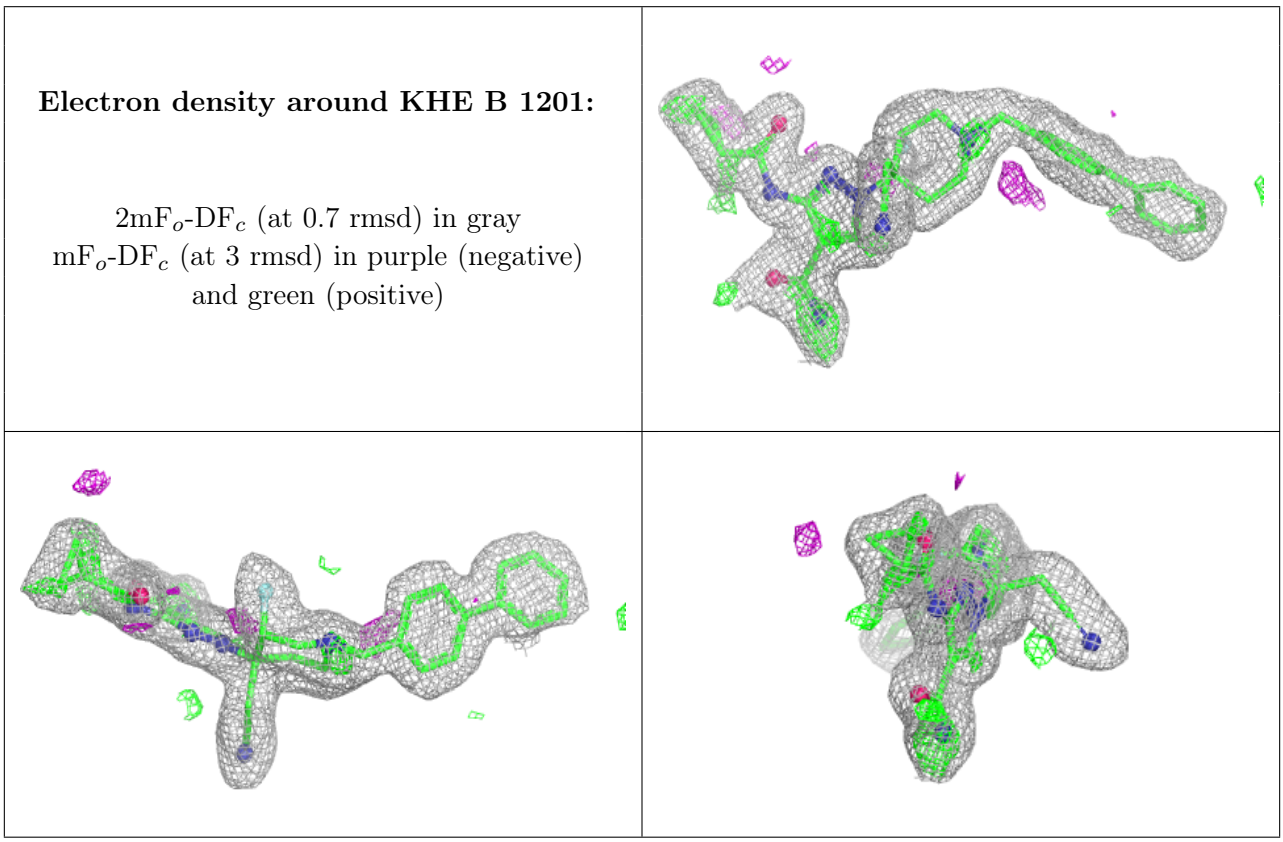
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	KHE	B	1201	37/37	0.93	0.13	11,18,31,33	0
2	KHE	A	1201	37/37	0.94	0.11	10,15,27,29	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.

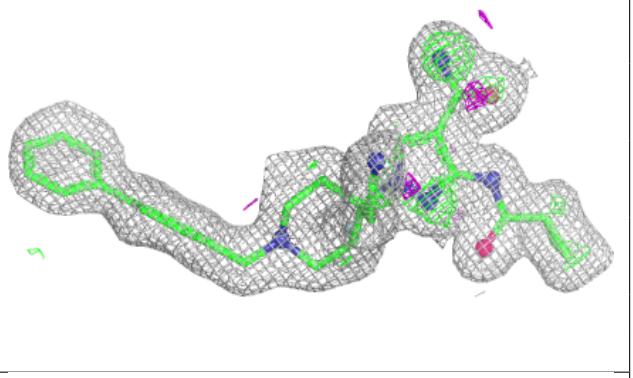
Electron density around KHE B 1201:

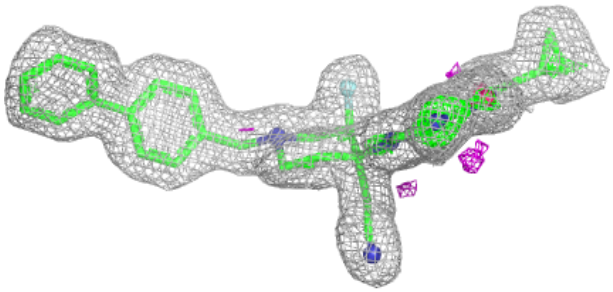
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

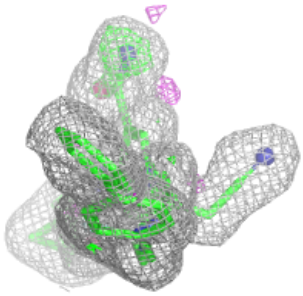


Electron density around KHE A 1201:

$2mF_o$-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.