



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:18 PM UTC

PDB ID : 6RSE / pdb_00006rse
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 : 1.80 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

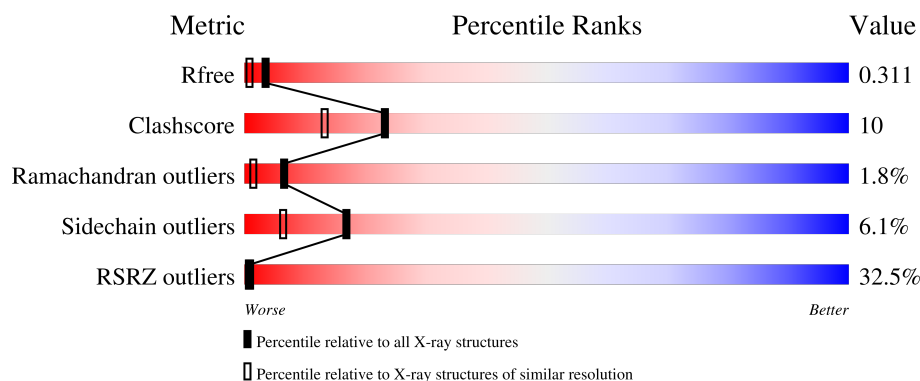
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	302	27% 72% 17% • • 5%
1	B	302	33% 69% 20% • • 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5000 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.

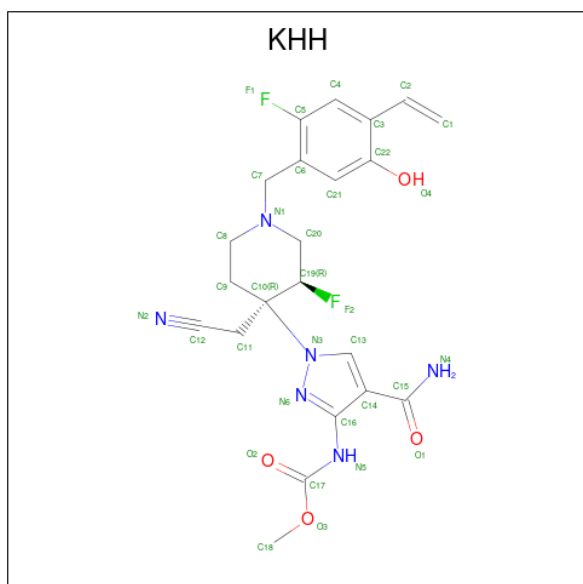
- Molecule 1 is a protein called Tyrosine-protein kinase JAK1.

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 methyl {N}-[4-aminocarbonyl-1-[(3 {R},4 {R})-4-(cyanomethyl)-1-[(4-ethenyl-2-fluoranyl-5-oxidanyl-phenyl)methyl]-3-fluoranyl-piperidin-4-yl]pyrazol-3-yl]carbamate (CCD ID: KHH) (formula: C₂₂H₂₄F₂N₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			34	22	2	6	4		
2	B	1	Total	C	F	N	O	0	0
			34	22	2	6	4		

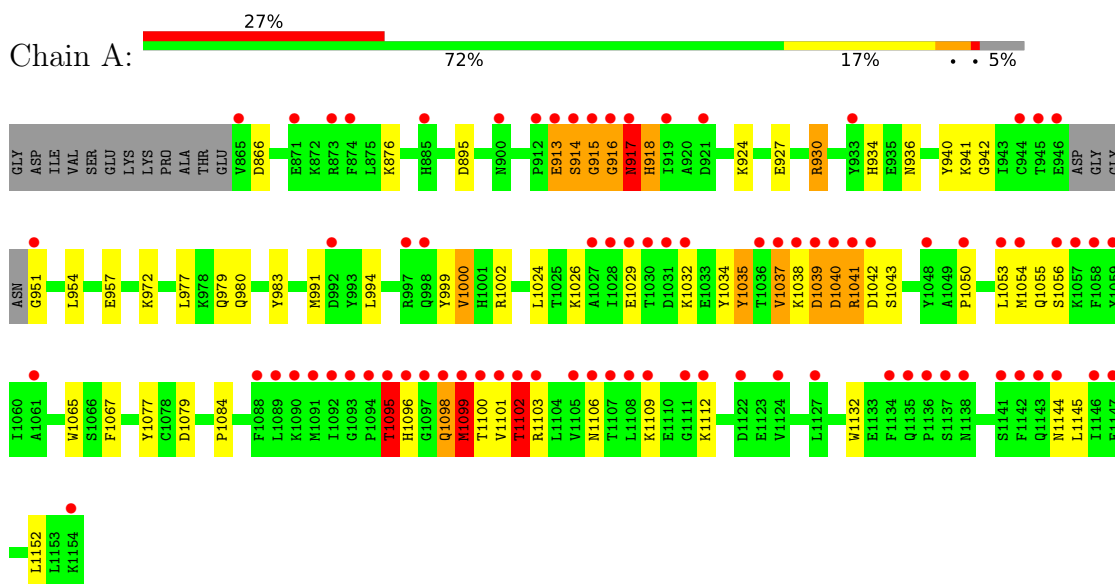
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	161	Total	O	0	0
			161	161		

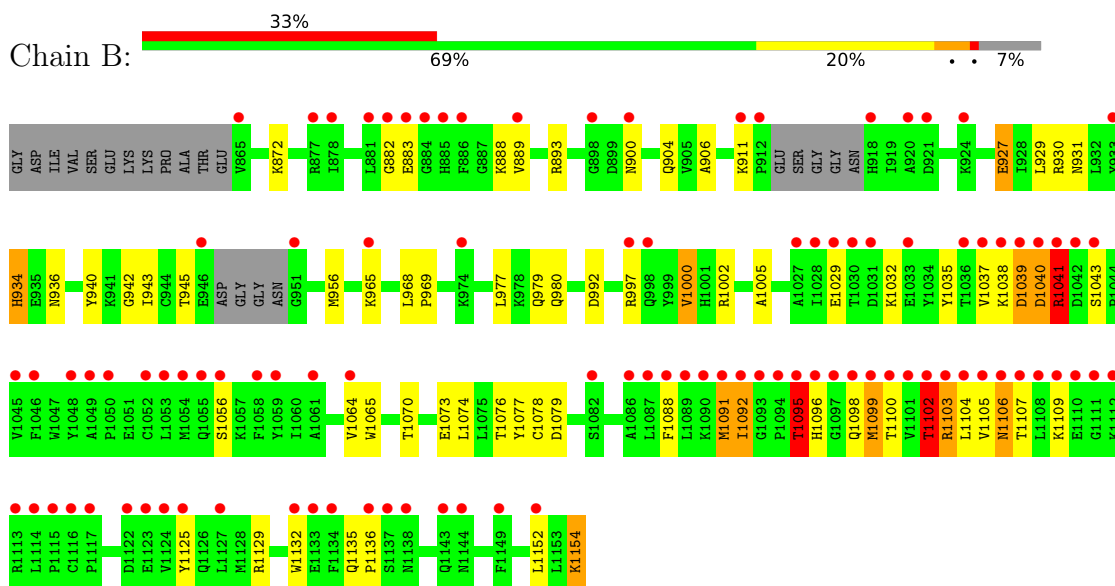
3 Residue-property plots [i](#)

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



• Molecule 1: Tyrosine-protein kinase JAK1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.89Å 88.96Å 173.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 1.80 39.04 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.04-1.80) 99.3 (39.04-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.263 , 0.303 0.270 , 0.311	Depositor DCC
R_{free} test set	3063 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5000	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 63.42 % 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 9.6906e-06. 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: PTR, KHH

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	1.26	9/2347 (0.4%)	1.48	11/3159 (0.3%)
1	B	1.49	20/2306 (0.9%)	1.46	6/3103 (0.2%)
All	All	1.38	29/4653 (0.6%)	1.47	17/6262 (0.3%)

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
1	B	0	3
All	All	0	6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1102	THR	C-O	24.36	1.54	1.24
1	B	1104	LEU	C-O	13.86	1.40	1.24
1	B	1105	VAL	C-O	12.50	1.39	1.24
1	B	1100	THR	C-O	10.00	1.35	1.24
1	B	1109	LYS	C-O	9.79	1.36	1.24
1	B	969	PRO	C-O	-7.85	1.14	1.24
1	B	956	MET	C-O	7.21	1.32	1.23
1	B	1102	THR	CA-C	6.98	1.62	1.52
1	A	1100	THR	C-O	6.97	1.32	1.24
1	A	1109	LYS	C-O	6.56	1.32	1.24
1	A	1026	LYS	C-O	6.26	1.31	1.23
1	B	1098	GLN	CA-C	6.21	1.61	1.52
1	B	1064	VAL	C-O	6.21	1.31	1.24
1	B	934	HIS	CE1-NE2	6.05	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1077	TYR	C-O	6.01	1.31	1.23
1	B	1099	MET	SD-CE	5.95	1.94	1.79
1	B	1099	MET	C-O	5.65	1.31	1.24
1	B	1076	THR	C-O	5.64	1.31	1.24
1	B	1005	ALA	C-O	5.63	1.30	1.23
1	A	1102	THR	CA-C	5.50	1.59	1.52
1	B	882	GLY	C-O	5.45	1.29	1.23
1	A	1099	MET	CG-SD	5.38	1.94	1.80
1	B	1092	ILE	N-CA	5.37	1.51	1.46
1	A	1084	PRO	C-O	-5.34	1.17	1.24
1	A	1145	LEU	C-O	5.33	1.30	1.24
1	B	1098	GLN	C-N	5.24	1.40	1.33
1	A	917	ASN	C-O	5.15	1.30	1.24
1	B	1073	GLU	N-CA	5.15	1.52	1.46
1	A	930	ARG	C-O	5.03	1.30	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1102	THR	CB-CA-C	8.09	123.78	110.92
1	A	991	MET	CA-C-O	-6.87	113.14	120.42
1	A	1079	ASP	CA-CB-CG	-6.63	105.97	112.60
1	A	1000	VAL	CB-CA-C	6.26	120.15	110.83
1	A	1102	THR	CA-C-O	-6.12	114.34	121.07
1	B	992	ASP	CA-CB-CG	-5.91	106.69	112.60
1	B	1105	VAL	O-C-N	5.77	127.69	121.87
1	B	1079	ASP	CA-CB-CG	-5.76	106.84	112.60
1	A	866	ASP	CB-CA-C	5.64	115.75	110.17
1	B	1070	THR	N-CA-C	-5.41	105.47	111.36
1	B	1000	VAL	CB-CA-C	5.38	118.85	110.83
1	A	1067	PHE	CA-C-O	-5.37	114.86	120.55
1	A	1040	ASP	CB-CA-C	-5.32	104.24	111.95
1	B	1095	THR	CB-CA-C	5.30	120.98	110.42
1	A	930	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	983	TYR	N-CA-C	-5.10	105.72	111.28
1	A	918	HIS	CA-C-O	-5.09	115.15	120.55

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1041	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	1102	THR	Mainchain
1	A	916	GLY	Peptide
1	B	1039	ASP	Peptide
1	B	1041	ARG	Peptide
1	B	1102	THR	Mainchain

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	2331	0	2315	54	0
1	B	2291	0	2286	54	0
2	A	34	0	0	0	0
2	B	34	0	0	0	0
3	A	149	0	0	7	0
3	B	161	0	0	6	0
All	All	5000	0	4601	96	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 10.

All (96) 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:B:900:ASN:HB2	3:B:1446:HOH:O	1.67	0.93
1:A:1103:ARG:HE	1:B:1041:ARG:HH22	1.08	0.91
1:A:1041:ARG:HH11	1:B:1096:HIS:CD2	1.90	0.90
1:B:906:ALA:HB1	3:B:1434:HOH:O	1.75	0.85
1:A:927:GLU:OE1	1:A:930:ARG:NH1	2.10	0.84
1:A:1099:MET:N	1:A:1099:MET:HE2	1.95	0.81
1:B:977:LEU:HA	1:B:980:GLN:HE21	1.45	0.79
1:A:977:LEU:HA	1:A:980:GLN:HE21	1.47	0.79
1:A:927:GLU:CD	1:A:930:ARG:NH1	2.44	0.75
1:A:1041:ARG:HH11	1:B:1096:HIS:CG	2.04	0.74
1:A:934:HIS:HD2	1:A:936:ASN:H	1.36	0.73
1:A:1098:GLN:C	1:A:1099:MET:HE2	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:HIS:HD2	1:B:936:ASN:H	1.38	0.72
1:A:927:GLU:OE2	1:A:930:ARG:NH1	2.21	0.71
1:A:1095:THR:HB	1:B:1040:ASP:HB3	1.72	0.71
1:A:927:GLU:OE2	3:A:1301:HOH:O	2.08	0.70
1:A:927:GLU:CD	1:A:930:ARG:HH12	1.99	0.70
1:A:1099:MET:HE2	1:A:1099:MET:CA	2.22	0.70
1:A:1032:LYS:NZ	1:A:1034:PTR:O2P	2.26	0.69
1:A:914:SER:HB2	1:A:918:HIS:HB2	1.75	0.68
1:A:1041:ARG:HH12	1:B:1103:ARG:HD2	1.57	0.68
1:A:1103:ARG:HE	1:B:1041:ARG:NH2	1.89	0.68
1:A:1041:ARG:NH1	1:B:1096:HIS:CD2	2.62	0.68
1:A:1103:ARG:NE	1:B:1041:ARG:HH22	1.89	0.66
1:A:1037:VAL:O	1:A:1056:SER:HB2	1.97	0.65
1:B:934:HIS:CD2	1:B:936:ASN:H	2.15	0.64
1:A:1053:LEU:O	1:B:1102:THR:HG21	1.97	0.64
1:A:934:HIS:CD2	1:A:936:ASN:H	2.15	0.63
1:A:954:LEU:HD13	3:A:1379:HOH:O	1.99	0.62
1:B:965:LYS:HD2	1:B:1078:CYS:HB3	1.80	0.62
1:A:1041:ARG:HH12	1:B:1103:ARG:CD	2.13	0.61
1:A:1035:PTR:HE1	1:A:1037:VAL:CG2	2.31	0.60
1:A:914:SER:HA	1:A:918:HIS:HD2	1.66	0.60
1:B:1039:ASP:O	1:B:1041:ARG:HD3	2.02	0.60
1:A:1035:PTR:HE1	1:A:1037:VAL:HG22	1.85	0.57
1:B:1041:ARG:HG3	1:B:1043:SER:HB3	1.85	0.57
1:B:904:GLN:NE2	3:B:1305:HOH:O	2.38	0.56
1:B:1029:GLU:OE2	1:B:1032:LYS:HE3	2.06	0.56
1:A:914:SER:CB	1:A:918:HIS:HB2	2.35	0.56
1:B:1041:ARG:HG3	1:B:1043:SER:CB	2.36	0.56
1:B:1065:TRP:CE3	1:B:1132:TRP:HA	2.42	0.54
1:A:940:TYR:CZ	1:A:942:GLY:HA2	2.45	0.52
1:B:1041:ARG:HG3	1:B:1043:SER:OG	2.10	0.51
1:B:1002:ARG:NH2	1:B:1037:VAL:HG21	2.25	0.51
1:A:915:GLY:O	1:A:917:ASN:N	2.43	0.51
1:A:951:GLY:C	3:A:1345:HOH:O	2.55	0.50
1:B:943:ILE:HD12	1:B:945:THR:CG2	2.42	0.50
1:B:893:ARG:NE	1:B:900:ASN:HD22	2.10	0.49
1:B:1154:LYS:HA	1:B:1154:LYS:CE	2.43	0.49
1:B:1029:GLU:OE2	1:B:1032:LYS:CE	2.60	0.49
1:A:954:LEU:CD1	3:A:1379:HOH:O	2.59	0.48
1:B:889:VAL:HG11	3:B:1434:HOH:O	2.12	0.48
1:A:1103:ARG:HH11	1:B:1041:ARG:NH2	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1040:ASP:OD1	1:B:1040:ASP:N	2.40	0.48
1:A:972:LYS:HE3	1:A:1077:TYR:CD2	2.49	0.47
1:B:1102:THR:O	1:B:1106:ASN:HB2	2.14	0.47
1:A:1102:THR:HG23	3:A:1311:HOH:O	2.13	0.47
1:A:1039:ASP:CG	1:A:1040:ASP:H	2.22	0.47
1:B:979:GLN:NE2	3:B:1314:HOH:O	2.48	0.47
1:B:893:ARG:NE	1:B:900:ASN:ND2	2.62	0.46
1:B:965:LYS:HE2	3:B:1441:HOH:O	2.15	0.46
1:A:1055:GLN:C	1:A:1056:SER:OG	2.58	0.46
1:A:941:LYS:HD2	1:A:957:GLU:HA	1.98	0.46
1:B:1092:ILE:O	1:B:1096:HIS:HE1	1.99	0.46
1:A:1041:ARG:HG3	1:A:1043:SER:OG	2.15	0.45
1:A:1035:PTR:CE1	1:A:1037:VAL:HG22	2.45	0.45
1:B:931:ASN:O	1:B:997:ARG:NH2	2.46	0.45
1:A:979:GLN:NE2	3:A:1310:HOH:O	2.49	0.45
1:B:1035:PTR:HE1	1:B:1037:VAL:HG22	1.98	0.45
1:A:1098:GLN:HE21	1:B:1041:ARG:HB3	1.81	0.44
1:A:1099:MET:HE2	1:A:1099:MET:HA	1.97	0.44
1:B:1125:TYR:CZ	1:B:1129:ARG:HD3	2.53	0.44
1:B:930:ARG:HG3	1:B:940:TYR:CE2	2.53	0.44
1:B:1039:ASP:O	1:B:1041:ARG:CD	2.65	0.44
1:B:1041:ARG:HD3	1:B:1041:ARG:N	2.33	0.44
1:B:980:GLN:O	1:B:1074:LEU:HD21	2.18	0.43
1:B:927:GLU:OE1	1:B:927:GLU:HA	2.18	0.43
1:A:1050:PRO:CB	1:A:1054:MET:HE2	2.48	0.43
1:B:940:TYR:CZ	1:B:942:GLY:HA2	2.53	0.43
1:B:943:ILE:HD12	1:B:945:THR:HG23	2.00	0.43
1:B:1088:PHE:HA	1:B:1091:MET:HE3	2.00	0.43
1:A:1099:MET:CA	1:A:1099:MET:CE	2.95	0.43
1:A:994:LEU:HG	1:A:999:TYR:HB2	2.01	0.42
1:B:1065:TRP:CZ3	1:B:1132:TRP:HA	2.54	0.42
1:B:1092:ILE:O	1:B:1096:HIS:CE1	2.72	0.42
1:A:1039:ASP:OD2	1:A:1040:ASP:N	2.44	0.42
1:A:1065:TRP:CE3	1:A:1132:TRP:HA	2.54	0.42
1:B:1135:GLN:HA	1:B:1136:PRO:HD2	1.93	0.42
1:A:940:TYR:HE2	3:A:1379:HOH:O	2.03	0.42
1:A:1002:ARG:NH1	1:A:1024:LEU:O	2.52	0.41
1:B:1091:MET:HE3	1:B:1091:MET:HB2	1.74	0.41
1:A:1029:GLU:HB3	1:A:1032:LYS:HG3	2.02	0.41
1:A:876:LYS:HE2	1:A:895:ASP:HB3	2.02	0.41
1:A:1101:VAL:O	1:A:1102:THR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:965:LYS:CD	1:B:1078:CYS:HB3	2.48	0.41
1:B:968:LEU:HD11	1:B:1074:LEU:HD12	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	281/302 (93%)	263 (94%)	9 (3%)	9 (3%)	3	0
1	B	273/302 (90%)	263 (96%)	9 (3%)	1 (0%)	30	19
All	All	554/604 (92%)	526 (95%)	18 (3%)	10 (2%)	6	1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	913	GLU
1	A	914	SER
1	A	916	GLY
1	A	1039	ASP
1	A	917	ASN
1	B	1095	THR
1	A	1095	THR
1	A	1096	HIS
1	A	1042	ASP
1	A	915	GLY

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%)	244 (95%)	12 (5%)	23	11
1	B	252/267 (94%)	233 (92%)	19 (8%)	12	4
All	All	508/534 (95%)	477 (94%)	31 (6%)	17	6

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	913	GLU
1	A	924	LYS
1	A	1000	VAL
1	A	1037	VAL
1	A	1038	LYS
1	A	1095	THR
1	A	1098	GLN
1	A	1099	MET
1	A	1106	ASN
1	A	1112	LYS
1	A	1144	ASN
1	A	1152	LEU
1	B	872	LYS
1	B	883	GLU
1	B	888	LYS
1	B	911	LYS
1	B	927	GLU
1	B	929	LEU
1	B	1000	VAL
1	B	1038	LYS
1	B	1040	ASP
1	B	1041	ARG
1	B	1056	SER
1	B	1091	MET
1	B	1095	THR
1	B	1099	MET
1	B	1103	ARG
1	B	1106	ASN
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 (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	934	HIS
1	A	936	ASN
1	A	971	ASN
1	A	979	GLN
1	A	980	GLN
1	A	1015	HIS
1	A	1098	GLN
1	A	1135	GLN
1	B	900	ASN
1	B	934	HIS
1	B	979	GLN
1	B	980	GLN
1	B	1096	HIS
1	B	1098	GLN
1	B	1106	ASN
1	B	1138	ASN
1	B	1144	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.64	0	17,22,24	0.72	0
1	PTR	A	1035	1	15,16,17	0.53	0	17,22,24	1.27	3 (17%)
1	PTR	B	1035	1	15,16,17	0.64	0	17,22,24	0.74	0
1	PTR	A	1034	1	15,16,17	0.62	0	17,22,24	0.68	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	PTR	B	1034	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1035	1	-	2/10/11/13	0/1/1/1
1	PTR	B	1035	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1034	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1035	PTR	O2P-P-OH	2.98	114.14	105.32
1	A	1035	PTR	OH-CZ-CE2	2.17	125.71	119.22
1	A	1035	PTR	OH-CZ-CE1	-2.08	112.97	119.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1035	PTR	CE1-CZ-OH-P
1	A	1035	PTR	CE2-CZ-OH-P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1035	PTR	3	0
1	B	1035	PTR	1	0
1	A	1034	PTR	1	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	KHH	A	1201	-	34,36,36	1.55	3 (8%)	38,52,52	2.05	9 (23%)
2	KHH	B	1201	-	34,36,36	1.15	1 (2%)	38,52,52	1.95	12 (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
2	KHH	A	1201	-	-	2/21/42/42	0/3/3/3
2	KHH	B	1201	-	-	2/21/42/42	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	KHH	C10-N3	-7.82	1.43	1.50
2	B	1201	KHH	C10-N3	-4.93	1.45	1.50
2	A	1201	KHH	C14-C16	-2.47	1.41	1.45
2	A	1201	KHH	C13-N3	2.14	1.37	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	KHH	C8-N1-C20	6.07	119.64	109.53
2	B	1201	KHH	C9-C10-C19	-5.13	99.48	108.83
2	A	1201	KHH	C7-N1-C8	4.57	120.91	111.07
2	B	1201	KHH	C8-N1-C20	4.57	117.13	109.53
2	A	1201	KHH	C7-N1-C20	4.17	118.09	111.27
2	B	1201	KHH	C13-N3-N6	-4.09	109.19	112.65
2	A	1201	KHH	C9-C10-C19	-3.97	101.59	108.83
2	A	1201	KHH	C6-C7-N1	3.71	119.33	112.75
2	B	1201	KHH	C7-N1-C8	3.64	118.89	111.07
2	A	1201	KHH	C13-N3-N6	-3.50	109.69	112.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	KHH	C7-N1-C20	3.28	116.64	111.27
2	B	1201	KHH	C10-N3-C13	3.03	132.27	128.71
2	A	1201	KHH	C10-N3-C13	2.97	132.20	128.71
2	A	1201	KHH	C9-C8-N1	2.89	114.10	111.16
2	B	1201	KHH	C9-C10-N3	-2.54	105.74	109.09
2	B	1201	KHH	O3-C17-N5	-2.30	106.50	109.15
2	A	1201	KHH	C14-C16-N6	-2.28	110.60	113.81
2	B	1201	KHH	C14-C16-N6	-2.22	110.68	113.81
2	B	1201	KHH	C6-C7-N1	2.15	116.56	112.75
2	B	1201	KHH	C13-C14-C15	2.14	130.98	125.03
2	B	1201	KHH	C9-C8-N1	2.04	113.24	111.16

There are no chirality outliers.

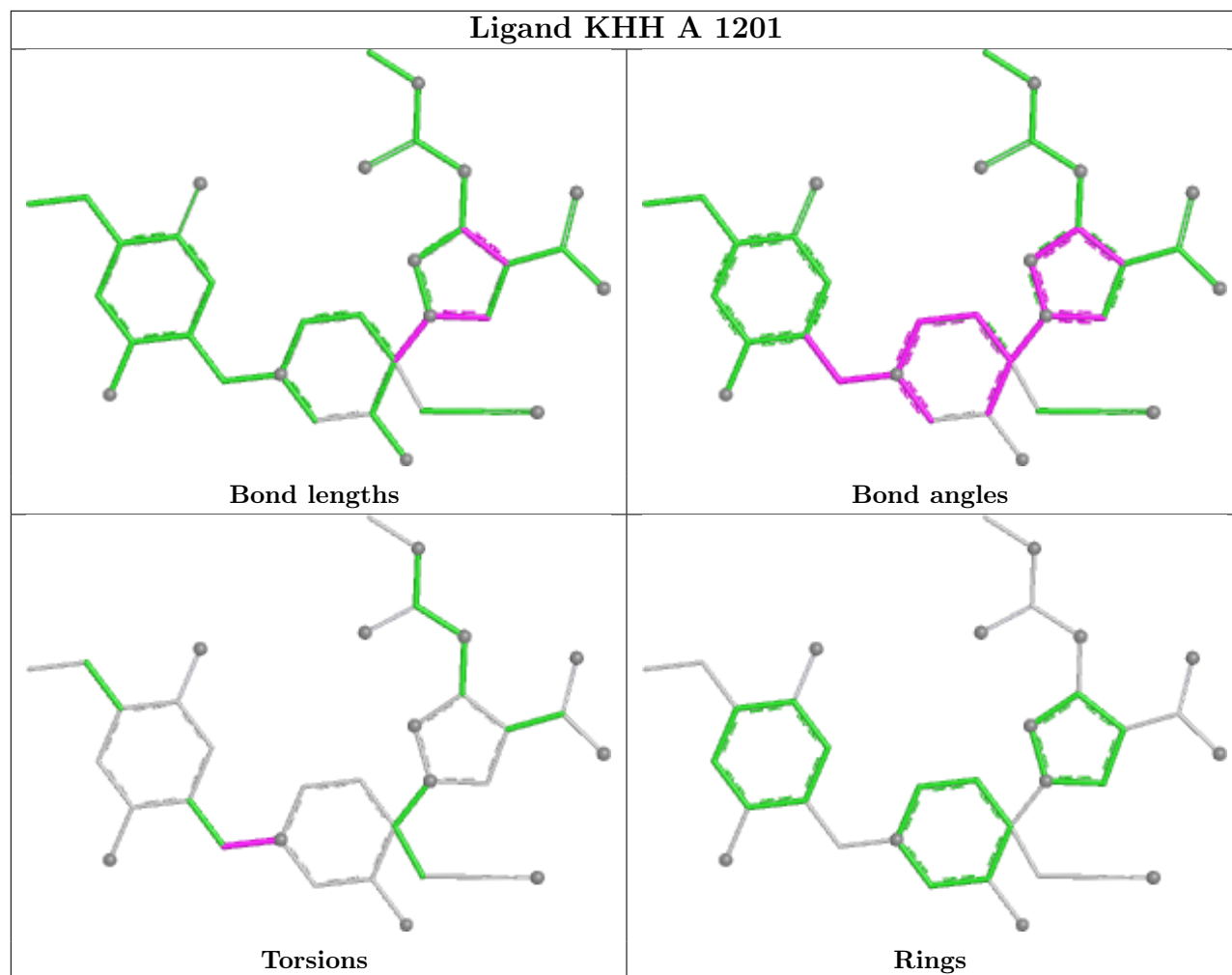
All (4) torsion outliers are listed below:

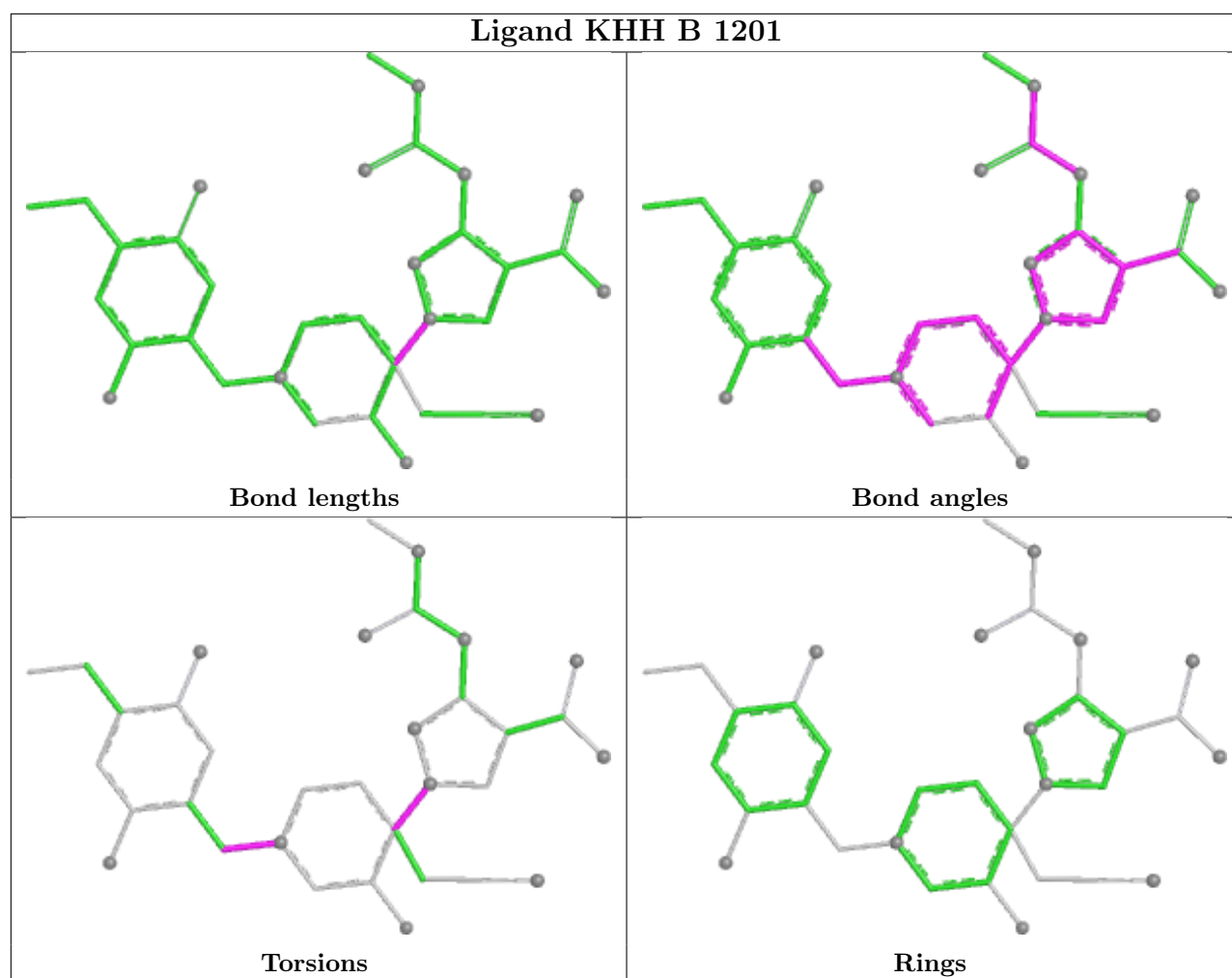
Mol	Chain	Res	Type	Atoms
2	A	1201	KHH	C6-C7-N1-C8
2	B	1201	KHH	C6-C7-N1-C20
2	B	1201	KHH	C11-C10-N3-N6
2	A	1201	KHH	C6-C7-N1-C20

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 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	284/302 (94%)	1.51	82 (28%) 1 1	14, 31, 62, 98	1 (0%)
1	B	279/302 (92%)	1.80	101 (36%) 1 0	16, 32, 65, 83	0
All	All	563/604 (93%)	1.65	183 (32%) 1 1	14, 32, 64, 98	1 (0%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1037	VAL	8.5
1	A	1095	THR	6.9
1	B	1037	VAL	6.3
1	B	1095	THR	5.6
1	B	1030	THR	5.6
1	B	1099	MET	5.4
1	A	917	ASN	5.4
1	B	1092	ILE	5.3
1	B	912	PRO	5.2
1	A	1039	ASP	5.1
1	B	1105	VAL	4.9
1	A	1038	LYS	4.8
1	B	1088	PHE	4.8
1	B	1093	GLY	4.7
1	B	1102	THR	4.7
1	B	1096	HIS	4.7
1	B	1104	LEU	4.7
1	B	1134	PHE	4.4
1	B	1039	ASP	4.4
1	B	1028	ILE	4.3
1	A	916	GLY	4.2
1	B	900	ASN	4.2
1	B	1138	ASN	4.2
1	B	1091	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	1137	SER	4.1
1	A	865	VAL	4.1
1	B	1107	THR	4.1
1	A	915	GLY	4.1
1	B	1101	VAL	4.0
1	B	1111	GLY	4.0
1	A	914	SER	4.0
1	B	1103	ARG	4.0
1	A	1098	GLN	4.0
1	A	1127	LEU	4.0
1	B	1087	LEU	4.0
1	B	1097	GLY	4.0
1	B	1123	GLU	4.0
1	B	1094	PRO	4.0
1	B	1108	LEU	3.9
1	A	1030	THR	3.9
1	B	1110	GLU	3.9
1	B	1098	GLN	3.9
1	B	1050	PRO	3.9
1	B	1152	LEU	3.8
1	A	1134	PHE	3.8
1	B	1106	ASN	3.7
1	B	865	VAL	3.7
1	B	1040	ASP	3.7
1	A	1092	ILE	3.7
1	A	951	GLY	3.7
1	A	933	TYR	3.7
1	A	1041	ARG	3.6
1	B	1124	VAL	3.6
1	A	1137	SER	3.5
1	B	1053	LEU	3.5
1	B	1100	THR	3.4
1	A	1111	GLY	3.4
1	B	1059	TYR	3.4
1	B	1058	PHE	3.4
1	A	1031	ASP	3.4
1	A	1102	THR	3.4
1	A	1036	THR	3.3
1	A	1100	THR	3.3
1	A	1054	MET	3.3
1	B	1086	ALA	3.3
1	B	946	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1109	LYS	3.3
1	A	1099	MET	3.3
1	A	885	HIS	3.3
1	A	1143	GLN	3.3
1	A	1040	ASP	3.3
1	B	1029	GLU	3.2
1	B	1048	TYR	3.2
1	B	886	PHE	3.2
1	A	1056	SER	3.2
1	B	965	LYS	3.2
1	B	885	HIS	3.2
1	B	878	ILE	3.2
1	A	1093	GLY	3.2
1	A	912	PRO	3.1
1	B	1114	LEU	3.1
1	B	1049	ALA	3.1
1	A	1136	PRO	3.1
1	A	1097	GLY	3.1
1	B	1090	LYS	3.1
1	A	946	GLU	3.1
1	A	1057	LYS	3.1
1	B	1054	MET	3.1
1	B	1082	SER	3.1
1	B	1061	ALA	3.1
1	B	1064	VAL	3.0
1	B	884	GLY	3.0
1	B	1112	LYS	3.0
1	A	1105	VAL	3.0
1	A	1090	LYS	3.0
1	A	1058	PHE	2.9
1	A	1108	LEU	2.9
1	B	1089	LEU	2.9
1	B	933	TYR	2.9
1	B	920	ALA	2.9
1	A	1042	ASP	2.9
1	B	1031	ASP	2.9
1	B	1042	ASP	2.9
1	A	1028	ILE	2.9
1	A	1142	PHE	2.8
1	A	1138	ASN	2.8
1	A	1144	ASN	2.8
1	A	1103	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	918	HIS	2.8
1	B	1038	LYS	2.8
1	A	1027	ALA	2.8
1	A	1101	VAL	2.8
1	A	1154	LYS	2.7
1	B	1036	THR	2.7
1	A	1094	PRO	2.7
1	A	1088	PHE	2.7
1	B	1122	ASP	2.7
1	B	924	LYS	2.7
1	A	873	ARG	2.6
1	A	1096	HIS	2.6
1	A	1109	LYS	2.6
1	A	1050	PRO	2.6
1	B	1041	ARG	2.6
1	B	1052	CYS	2.6
1	A	1053	LEU	2.6
1	A	1091	MET	2.6
1	A	997	ARG	2.5
1	B	1125	TYR	2.5
1	A	1107	THR	2.5
1	A	1048	TYR	2.5
1	B	921	ASP	2.5
1	A	998	GLN	2.5
1	B	1127	LEU	2.5
1	A	919	ILE	2.5
1	B	1055	GLN	2.5
1	A	945	THR	2.5
1	B	1056	SER	2.4
1	A	1106	ASN	2.4
1	A	1029	GLU	2.4
1	A	1059	TYR	2.4
1	B	1113	ARG	2.4
1	B	1045	VAL	2.4
1	B	881	LEU	2.4
1	B	974	LYS	2.4
1	A	913	GLU	2.4
1	B	1136	PRO	2.4
1	B	877	ARG	2.3
1	A	871	GLU	2.3
1	B	1115	PRO	2.3
1	A	1032	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1132	TRP	2.3
1	A	1061	ALA	2.3
1	A	1112	LYS	2.3
1	B	997	ARG	2.3
1	A	921	ASP	2.3
1	B	1133	GLU	2.3
1	A	1089	LEU	2.3
1	B	883	GLU	2.2
1	B	1033	GLU	2.2
1	B	1117	PRO	2.2
1	A	1141	SER	2.2
1	B	898	GLY	2.2
1	B	1027	ALA	2.2
1	A	874	PHE	2.2
1	B	1149	PHE	2.2
1	B	889	VAL	2.2
1	A	1147	GLU	2.2
1	A	1124	VAL	2.2
1	A	1135	GLN	2.2
1	B	1116	CYS	2.1
1	B	998	GLN	2.1
1	B	1043	SER	2.1
1	A	944	CYS	2.1
1	B	1143	GLN	2.1
1	B	1046	PHE	2.1
1	A	992	ASP	2.1
1	A	1122	ASP	2.1
1	A	1146	ILE	2.1
1	A	900	ASN	2.1
1	B	911	LYS	2.0
1	B	951	GLY	2.0
1	B	1144	ASN	2.0
1	B	882	GLY	2.0

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

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($\text{\AA}^2$)	Q<0.9
1	PTR	B	1034	16/17	0.75	0.18	52,62,73,75	0
1	PTR	A	1035	16/17	0.79	0.16	39,48,63,64	0
1	PTR	B	1035	16/17	0.79	0.17	46,54,67,67	0
1	PTR	A	1034	16/17	0.80	0.17	45,54,67,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

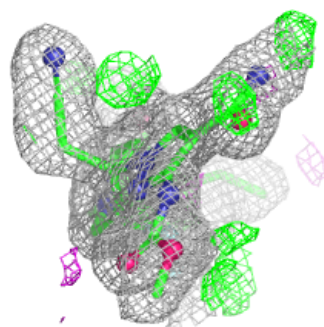
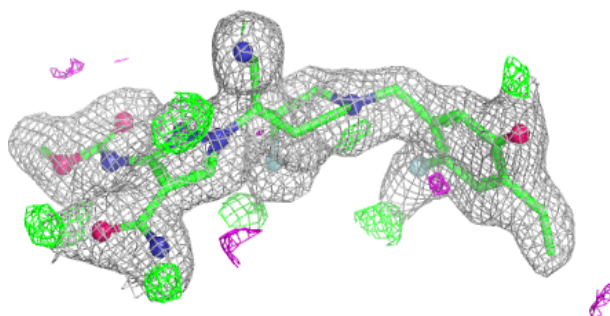
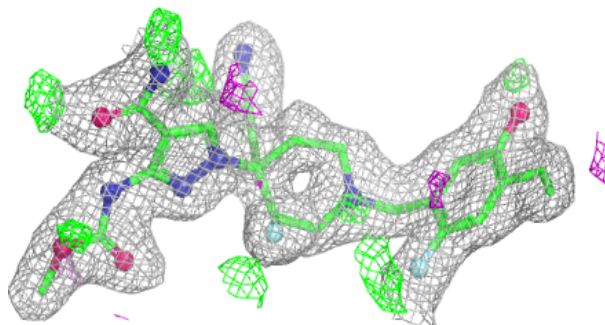
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KHH	B	1201	34/34	0.92	0.09	17,21,31,31	0
2	KHH	A	1201	34/34	0.94	0.07	16,19,29,31	0

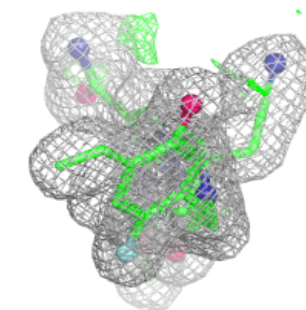
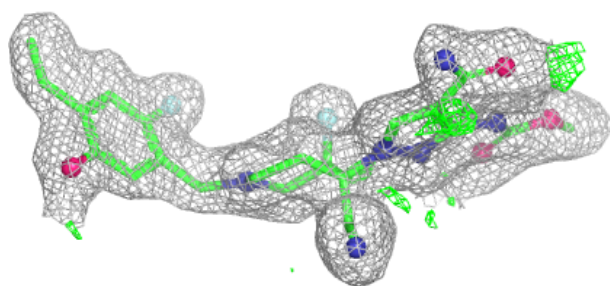
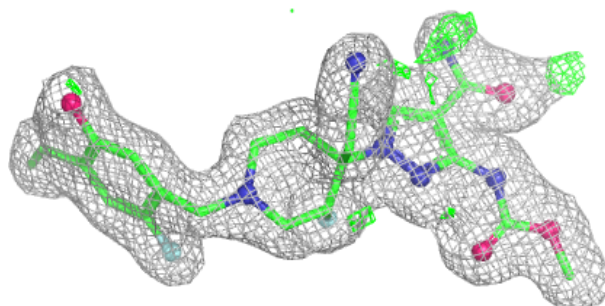
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KHH 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 KHH 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.