Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 12:23 AM EDT

PDB ID	:	4EHZ
Title	:	The Jak1 kinase domain in complex with inhibitor
Authors	:	Lupardus, P.J.; Steffek, M.
Deposited on	:	2012-04-04
Resolution	:	2.17 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

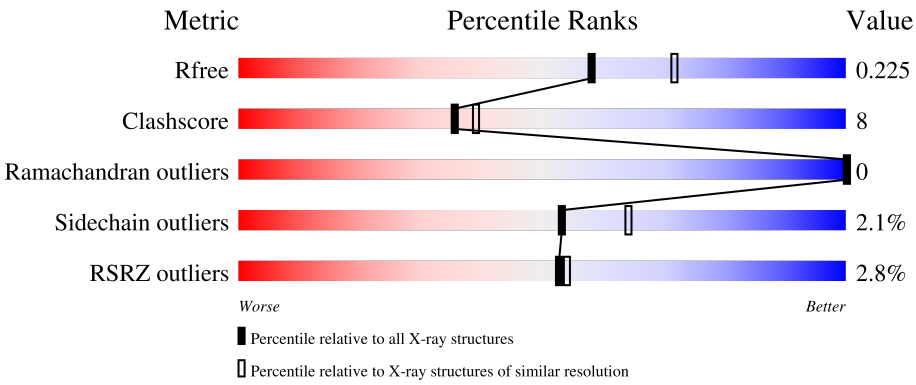
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.17 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	4% 77% 17% • •
1	B	302	2% 80% 12% • 7%
1	C	302	2% 82% 10% • 7%
1	D	302	2% 77% 15% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	C	1205	-	-	X	-
3	EDO	D	1203	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9938 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.

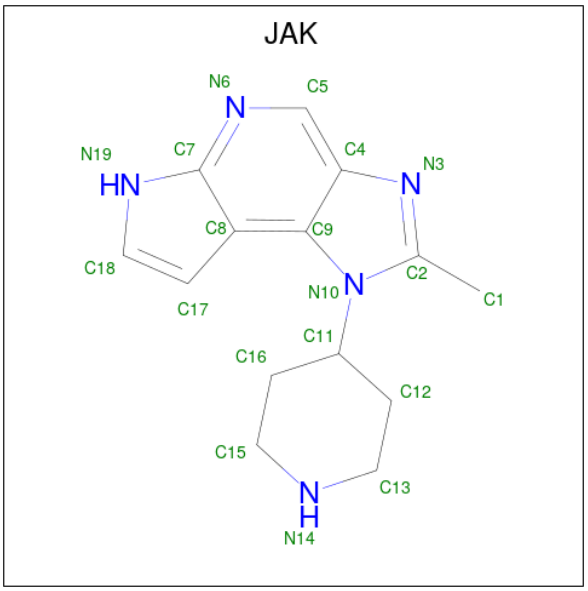
- Molecule 1 is a protein called Tyrosine-protein kinase JAK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	292	2363	1504	402	440	2	15	0	0	0
1	B	282	2304	1469	392	426	2	15	0	1	0
1	C	280	2288	1459	390	422	2	15	0	1	0
1	D	282	2298	1464	391	426	2	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

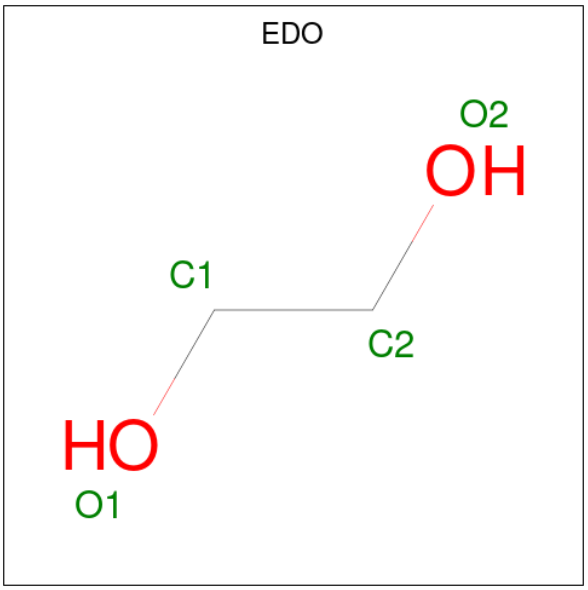
Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	-	EXPRESSION TAG	UNP P23458
B	853	GLY	-	EXPRESSION TAG	UNP P23458
C	853	GLY	-	EXPRESSION TAG	UNP P23458
D	853	GLY	-	EXPRESSION TAG	UNP P23458

- Molecule 2 is 2-methyl-1-(piperidin-4-yl)-1,6-dihydroimidazo[4,5-d]pyrrolo[2,3-b]pyridine (three-letter code: JAK) (formula: $C_{14}H_{17}N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	19	14	5	0	0
2	B	1	19	14	5	0	0
2	C	1	19	14	5	0	0
2	D	1	19	14	5	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0

- Molecule 4 is water.

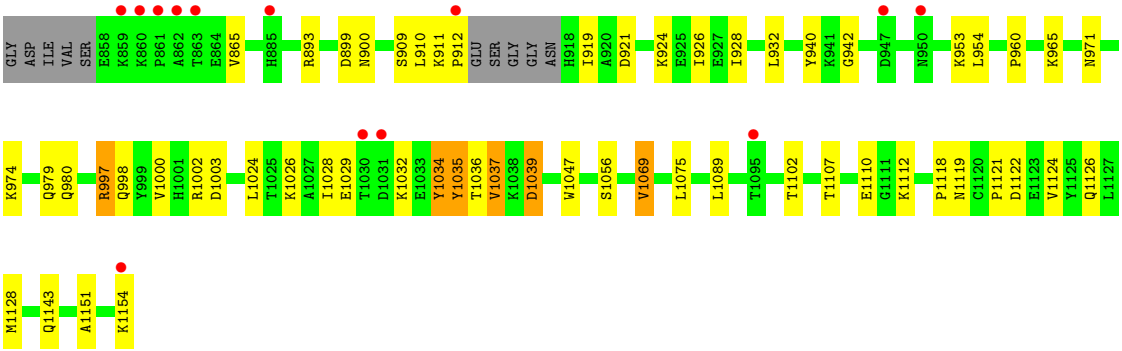
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	136	136	136	0	0
			Total	O		
4	B	132	132	132	0	0
			Total	O		
4	C	166	166	166	0	0
			Total	O		
4	D	127	127	127	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

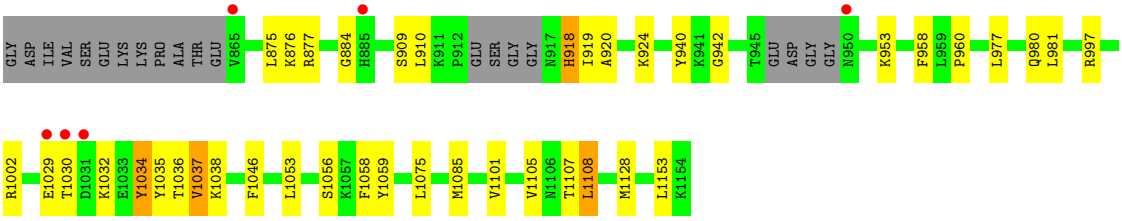
• Molecule 1: Tyrosine-protein kinase JAK1

Chain A:



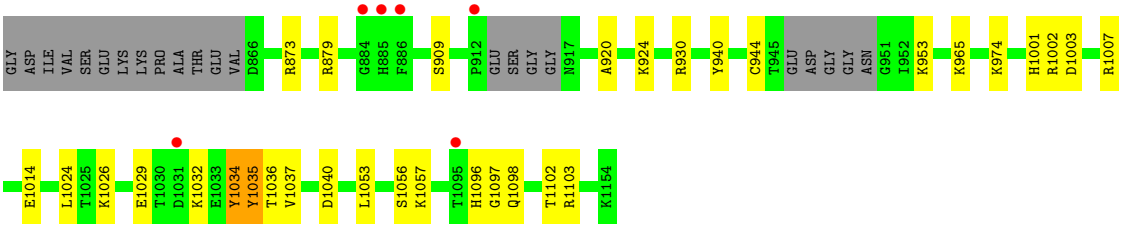
• Molecule 1: Tyrosine-protein kinase JAK1

Chain B:



• Molecule 1: Tyrosine-protein kinase JAK1

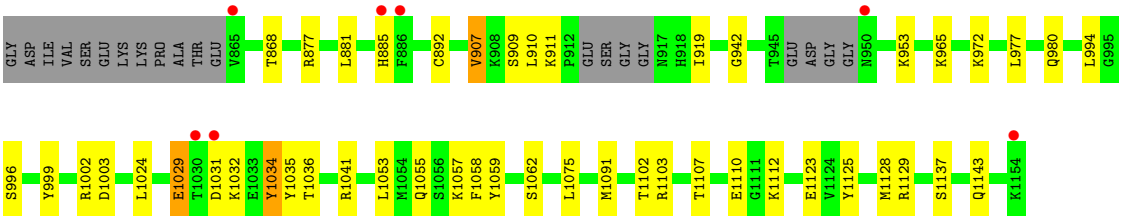
Chain C:



• Molecule 1: Tyrosine-protein kinase JAK1

Chain D:

2%
77%
15%
7%


GLY ASP ILE VAL SER GLU LYS LYS PRO ALA THR GLU V865 T868 R877 L881 H885 F886 C892 V907 K908 S909 L910 K911 P912 GLU SER GLY GLY N917 H918 I919 G942 T945 GLU ASP GLY GLY N950 K953 K965 K972 L977 Q980 L994 G995
S996 Y999 R1002 D1003 L1024 E1029 T1030 D1031 K1032 E1033 Y1034 Y1035 T1036 R1041 L1053 M1054 Q1055 S1056 K1057 F1058 Y1059 S1062 L1075 M1091 T1102 R1103 T1107 E1110 G1111 K1112 E1123 V1124 Y1125 M1128 R1129 S1137 Q1143 K1154

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.71Å 172.18Å 88.03Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	30.00 – 2.17 30.04 – 2.17	Depositor EDS
% Data completeness (in resolution range)	90.7 (30.00-2.17) 95.4 (30.04-2.17)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_648)	Depositor
R, R_{free}	0.171 , 0.229 0.172 , 0.225	Depositor DCC
R_{free} test set	3211 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9938	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 43.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6448e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: JAK, EDO, 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	0.38	0/2380	0.54	0/3204
1	B	0.38	0/2322	0.53	0/3124
1	C	0.41	0/2306	0.55	0/3102
1	D	0.39	0/2313	0.53	0/3113
All	All	0.39	0/9321	0.54	0/12543

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2363	0	2354	45	0
1	B	2304	0	2305	29	0
1	C	2288	0	2286	40	0
1	D	2298	0	2292	41	0
2	A	19	0	17	0	0
2	B	19	0	17	1	0
2	C	19	0	17	1	0
2	D	19	0	17	1	0
3	A	20	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	6	0	0
3	C	16	0	24	10	0
3	D	8	0	12	5	0
4	A	136	0	0	1	0
4	B	132	0	0	1	0
4	C	166	0	0	2	0
4	D	127	0	0	3	0
All	All	9938	0	9377	151	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 8.

All (151) 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:C:879:ARG:HH22	3:C:1202:EDO:H12	1.40	0.86
1:C:965:LYS:HD2	1:C:1007[B]:ARG:HB3	1.57	0.85
1:C:965:LYS:HD2	1:C:1007[A]:ARG:HB3	1.61	0.81
1:D:972:LYS:N	3:D:1203:EDO:H12	1.96	0.81
1:C:1056:SER:HA	3:C:1205:EDO:H21	1.62	0.79
1:C:965:LYS:HZ2	1:C:1007[A]:ARG:H	1.28	0.79
1:D:1107:THR:HG23	1:D:1112:LYS:HD2	1.63	0.78
1:C:965:LYS:HZ2	1:C:1007[B]:ARG:H	1.29	0.78
1:D:868:THR:HG21	4:D:1417:HOH:O	1.84	0.78
1:B:1029:GLU:HG2	1:B:1032:LYS:HB2	1.67	0.76
1:D:972:LYS:HB2	3:D:1203:EDO:H11	1.70	0.72
1:D:877:ARG:HH22	1:D:953:LYS:HE3	1.57	0.70
1:A:1037:VAL:HG12	1:A:1056:SER:OG	1.92	0.70
1:C:1029:GLU:HB3	1:C:1032:LYS:HE2	1.72	0.69
1:C:1035:PTR:HE1	1:C:1037:VAL:HG22	1.75	0.68
1:D:1110:GLU:OE1	1:D:1112:LYS:HE2	1.95	0.67
1:A:1002:ARG:NH2	1:A:1037:VAL:HG21	2.10	0.67
1:B:1029:GLU:HG3	1:B:1032:LYS:HD3	1.77	0.67
1:D:885:HIS:O	1:D:911:LYS:HE3	1.96	0.65
1:D:909:SER:HB3	1:D:953:LYS:HG2	1.78	0.64
1:C:965:LYS:NZ	1:C:1007[A]:ARG:H	1.95	0.63
1:A:924:LYS:NZ	1:A:1026:LYS:NZ	2.46	0.62
1:C:965:LYS:NZ	1:C:1007[B]:ARG:H	1.95	0.62
1:C:1040:ASP:CB	3:C:1205:EDO:H11	2.30	0.62
1:B:920:ALA:O	1:B:924:LYS:HE2	1.98	0.62
1:C:1040:ASP:HB3	3:C:1205:EDO:H11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:LYS:HZ1	1:A:1026:LYS:NZ	1.98	0.62
1:D:1075:LEU:HD12	1:D:1128:MET:HE1	1.80	0.61
1:D:1002:ARG:HA	1:D:1058:PHE:CZ	2.35	0.61
1:A:921:ASP:O	1:A:924:LYS:HG2	2.00	0.61
1:A:1047:TRP:CD1	1:A:1069:VAL:HG22	2.37	0.59
1:A:1107:THR:HG22	1:A:1112:LYS:HB2	1.85	0.58
1:B:1002:ARG:HA	1:B:1058:PHE:CZ	2.38	0.58
1:C:879:ARG:HH22	3:C:1202:EDO:C1	2.15	0.58
1:B:1038:LYS:N	1:B:1038:LYS:HD2	2.19	0.57
1:A:1002:ARG:HD3	1:A:1024:LEU:O	2.05	0.56
1:A:1032:LYS:N	1:A:1032:LYS:HD2	2.20	0.56
1:D:1031:ASP:O	1:D:1032:LYS:HG3	2.05	0.56
1:B:876:LYS:HE2	1:D:996:SER:HA	1.86	0.56
1:A:928:ILE:O	1:A:932:LEU:HG	2.05	0.56
1:C:1056:SER:CA	3:C:1205:EDO:H21	2.32	0.56
1:C:1002:ARG:HH11	1:C:1026:LYS:HD3	1.70	0.56
1:C:920:ALA:O	1:C:924:LYS:HE2	2.06	0.55
1:A:1029:GLU:HG2	1:A:1032:LYS:HD3	1.88	0.55
1:B:1034:PTR:HE2	1:B:1036:THR:OG1	2.07	0.55
1:A:1110:GLU:HB3	1:A:1112:LYS:NZ	2.22	0.55
1:D:885:HIS:CE1	1:D:1041:ARG:NH2	2.75	0.55
1:A:924:LYS:HZ1	1:A:1026:LYS:CE	2.19	0.55
1:D:972:LYS:H	3:D:1203:EDO:H12	1.72	0.55
1:D:1034:PTR:HE2	1:D:1036:THR:OG1	2.07	0.54
1:D:977:LEU:HA	1:D:980:GLN:OE1	2.07	0.54
1:A:1000:VAL:HG13	1:A:1028:ILE:HD11	1.89	0.54
1:A:926:ILE:HG12	1:A:954:LEU:HD13	1.91	0.53
1:A:1039:ASP:OD1	1:A:1039:ASP:C	2.47	0.53
1:D:1029:GLU:HB3	1:D:1032:LYS:HD2	1.91	0.53
1:C:944:CYS:HB3	1:C:953:LYS:HB2	1.90	0.52
1:B:884:GLY:HA3	4:B:1428:HOH:O	2.09	0.52
1:D:965:LYS:HE2	4:D:1411:HOH:O	2.09	0.52
1:D:910:LEU:HD11	1:D:919:ILE:HA	1.89	0.52
1:A:980:GLN:HE22	3:A:1203:EDO:H12	1.75	0.52
1:C:1026:LYS:HG2	1:C:1035:PTR:CZ	2.40	0.52
1:D:972:LYS:HB2	3:D:1203:EDO:C1	2.40	0.52
1:A:979:GLN:HB2	3:A:1206:EDO:H11	1.91	0.52
1:A:1035:PTR:HE1	1:A:1037:VAL:HG23	1.91	0.51
1:B:1075:LEU:HD12	1:B:1128:MET:HE1	1.92	0.51
1:C:1003:ASP:HB2	1:C:1024:LEU:HD12	1.92	0.51
1:C:1056:SER:HA	3:C:1205:EDO:C2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1053:LEU:O	1:D:1102:THR:HG21	2.11	0.50
1:C:1007[A]:ARG:HD3	4:C:1403:HOH:O	2.10	0.50
1:B:910:LEU:HD11	1:B:919:ILE:HA	1.94	0.50
1:C:965:LYS:HE2	4:C:1403:HOH:O	2.13	0.49
1:C:1102:THR:HG21	1:D:1053:LEU:O	2.13	0.49
1:B:924:LYS:N	1:B:924:LYS:HD3	2.27	0.49
1:B:1046:PHE:CE2	1:B:1085:MET:HG3	2.48	0.49
1:A:1151:ALA:HA	1:A:1154:LYS:HE2	1.93	0.49
1:A:924:LYS:NZ	1:A:1026:LYS:HZ2	2.10	0.48
1:D:1057:LYS:HD3	1:D:1059:TYR:OH	2.12	0.48
1:D:868:THR:HG23	1:D:942:GLY:HA2	1.95	0.48
1:D:1107:THR:HG22	1:D:1112:LYS:HB2	1.95	0.48
1:A:1039:ASP:OD1	1:A:1039:ASP:O	2.31	0.48
1:C:1002:ARG:NH1	1:C:1026:LYS:HD3	2.28	0.48
1:B:1034:PTR:HD1	1:B:1059:TYR:CE2	2.49	0.48
1:A:1110:GLU:HB3	1:A:1112:LYS:HZ3	1.78	0.48
1:C:1026:LYS:HG2	1:C:1035:PTR:CE1	2.43	0.48
1:A:1118:PRO:O	1:A:1119:ASN:HB2	2.14	0.48
1:C:1056:SER:CB	3:C:1205:EDO:H21	2.44	0.48
1:C:1097:GLY:N	1:D:1041:ARG:HG3	2.29	0.47
1:B:940:TYR:CZ	1:B:942:GLY:HA2	2.50	0.47
1:B:1029:GLU:H	1:B:1029:GLU:CD	2.16	0.47
1:A:1122:ASP:O	1:A:1126:GLN:HG2	2.14	0.47
1:A:1037:VAL:HG11	4:A:1416:HOH:O	2.15	0.47
1:B:981:LEU:HB2	1:B:1153:LEU:HD21	1.96	0.47
1:C:909:SER:HB3	1:C:953:LYS:HG2	1.97	0.47
1:C:1034:PTR:CZ	1:C:1057:LYS:HE3	2.45	0.47
1:C:1040:ASP:HB2	3:C:1205:EDO:H11	1.97	0.46
1:D:1058:PHE:CE1	1:D:1062:SER:HB2	2.50	0.46
1:D:994:LEU:HG	1:D:999:TYR:HB2	1.96	0.46
1:A:893:ARG:NE	1:A:900:ASN:ND2	2.63	0.46
1:B:920:ALA:O	1:B:924:LYS:HG2	2.15	0.46
1:A:909:SER:HB3	1:A:953:LYS:HG2	1.97	0.46
1:A:1003:ASP:HB2	1:A:1024:LEU:HD12	1.96	0.46
1:A:940:TYR:CZ	1:A:942:GLY:HA2	2.50	0.46
1:B:1037:VAL:HG13	1:B:1056:SER:O	2.15	0.46
1:B:977:LEU:HA	1:B:980:GLN:OE1	2.17	0.45
2:B:1201:JAK:H1	2:B:1201:JAK:H11	1.85	0.45
1:C:1040:ASP:OD2	1:D:1103:ARG:NH1	2.49	0.45
1:D:965:LYS:HE3	4:D:1324:HOH:O	2.16	0.45
1:B:1101:VAL:O	1:B:1105:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1201:JAK:H1	2:D:1201:JAK:H11	1.84	0.45
1:A:910:LEU:HD11	1:A:919:ILE:HA	1.99	0.45
1:C:1096:HIS:CD2	1:C:1103:ARG:HG3	2.53	0.44
1:D:972:LYS:N	3:D:1203:EDO:C1	2.75	0.44
1:A:1102:THR:HG21	1:B:1053:LEU:O	2.17	0.44
1:B:909:SER:HB3	1:B:953:LYS:HG2	2.00	0.44
1:B:1108:LEU:HD12	1:B:1108:LEU:HA	1.89	0.44
1:C:1032:LYS:HB2	1:C:1032:LYS:HZ3	1.83	0.44
1:D:1034:PTR:HE1	1:D:1034:PTR:O3P	2.17	0.43
1:D:1057:LYS:HE2	1:D:1057:LYS:HB3	1.85	0.43
1:A:1034:PTR:HE2	1:A:1036:THR:OG1	2.19	0.43
1:A:997:ARG:O	1:A:998:GLN:HB2	2.19	0.43
1:D:885:HIS:C	1:D:911:LYS:HE3	2.38	0.43
1:B:1029:GLU:CG	1:B:1032:LYS:HD3	2.45	0.43
1:C:930:ARG:HG2	1:C:940:TYR:CZ	2.53	0.43
1:B:1034:PTR:HD2	1:B:1034:PTR:C	2.48	0.43
1:A:971:ASN:OD1	1:A:974:LYS:HD3	2.19	0.43
1:A:1034:PTR:CD2	1:A:1034:PTR:C	2.97	0.42
1:D:1091:MET:HE2	1:D:1107:THR:HG21	2.01	0.42
1:A:960:PRO:O	3:A:1202:EDO:H11	2.20	0.42
1:D:892:CYS:SG	1:D:907:VAL:CG1	3.07	0.42
1:A:1107:THR:CG2	1:A:1112:LYS:HB2	2.48	0.42
1:B:877:ARG:NH2	1:D:1137:SER:O	2.52	0.42
1:C:1034:PTR:O3P	1:C:1034:PTR:HE1	2.20	0.42
1:A:1032:LYS:N	1:A:1032:LYS:CD	2.81	0.42
1:D:877:ARG:NH2	1:D:953:LYS:HE3	2.30	0.42
1:C:1001:HIS:O	1:C:1002:ARG:HB2	2.20	0.42
1:D:1125:TYR:CZ	1:D:1129:ARG:HD3	2.55	0.42
1:A:1075:LEU:HD12	1:A:1128:MET:HE1	2.02	0.41
1:A:1121:PRO:HG2	1:A:1124:VAL:HG23	2.01	0.41
1:D:1003:ASP:HB2	1:D:1024:LEU:HD12	2.02	0.41
1:D:1059:TYR:CD1	1:D:1059:TYR:N	2.88	0.41
1:B:918:HIS:ND1	1:B:918:HIS:N	2.67	0.41
1:A:1075:LEU:HD12	1:A:1128:MET:CE	2.51	0.41
1:A:1089:LEU:HD23	1:A:1089:LEU:HA	1.83	0.41
1:C:1098:GLN:HA	3:C:1203:EDO:H11	2.02	0.41
1:A:911:LYS:HA	1:A:912:PRO:HD3	1.89	0.40
1:B:875:LEU:HD12	1:B:875:LEU:HA	1.94	0.40
1:A:899:ASP:O	1:A:900:ASN:HB3	2.20	0.40
1:C:974:LYS:HD3	1:C:1014:GLU:OE1	2.21	0.40
1:B:958:PHE:CZ	1:B:960:PRO:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1201:JAK:H11	2:C:1201:JAK:H1	1.83	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	286/302 (95%)	277 (97%)	9 (3%)	0	100	100
1	B	275/302 (91%)	270 (98%)	5 (2%)	0	100	100
1	C	273/302 (90%)	265 (97%)	8 (3%)	0	100	100
1	D	274/302 (91%)	270 (98%)	4 (2%)	0	100	100
All	All	1108/1208 (92%)	1082 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	258/267 (97%)	251 (97%)	7 (3%)	44	54
1	B	254/267 (95%)	248 (98%)	6 (2%)	49	59
1	C	251/267 (94%)	249 (99%)	2 (1%)	81	89
1	D	253/267 (95%)	247 (98%)	6 (2%)	49	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1016/1068 (95%)	995 (98%)	21 (2%)	53 64

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	865	VAL
1	A	965	LYS
1	A	997	ARG
1	A	1037	VAL
1	A	1039	ASP
1	A	1069	VAL
1	A	1143	GLN
1	B	918	HIS
1	B	997	ARG
1	B	1030	THR
1	B	1037	VAL
1	B	1107	THR
1	B	1108	LEU
1	C	873	ARG
1	C	1036	THR
1	D	881	LEU
1	D	907	VAL
1	D	1029	GLU
1	D	1055	GLN
1	D	1123	GLU
1	D	1143	GLN

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

Mol	Chain	Res	Type
1	A	900	ASN
1	A	950	ASN
1	C	1096	HIS
1	D	869	HIS
1	D	885	HIS
1	D	1055	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	D	1034	1	15,16,17	1.90	1 (6%)	17,22,24	0.73	0
1	PTR	A	1035	1	15,16,17	1.85	1 (6%)	17,22,24	0.66	0
1	PTR	C	1034	1	15,16,17	1.96	1 (6%)	17,22,24	0.87	1 (5%)
1	PTR	B	1034	1	15,16,17	1.98	1 (6%)	17,22,24	0.68	0
1	PTR	D	1035	1	15,16,17	1.90	1 (6%)	17,22,24	0.65	0
1	PTR	B	1035	1	15,16,17	1.83	1 (6%)	17,22,24	0.65	0
1	PTR	C	1035	1	15,16,17	1.88	1 (6%)	17,22,24	0.67	0
1	PTR	A	1034	1	15,16,17	1.95	1 (6%)	17,22,24	0.85	1 (5%)

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	D	1034	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1035	1	-	0/10/11/13	0/1/1/1
1	PTR	C	1034	1	-	2/10/11/13	0/1/1/1
1	PTR	B	1034	1	-	0/10/11/13	0/1/1/1
1	PTR	D	1035	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1035	1	-	0/10/11/13	0/1/1/1
1	PTR	C	1035	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1034	1	-	0/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1034	PTR	OH-CZ	-7.49	1.23	1.40
1	C	1034	PTR	OH-CZ	-7.25	1.24	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1034	PTR	OH-CZ	-7.21	1.24	1.40
1	D	1035	PTR	OH-CZ	-7.09	1.24	1.40
1	D	1034	PTR	OH-CZ	-7.05	1.24	1.40
1	C	1035	PTR	OH-CZ	-6.94	1.25	1.40
1	A	1035	PTR	OH-CZ	-6.78	1.25	1.40
1	B	1035	PTR	OH-CZ	-6.66	1.25	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1034	PTR	O3P-P-OH	2.65	113.16	105.32
1	A	1034	PTR	O3P-P-OH	2.29	112.09	105.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1034	PTR	CZ-OH-P-O1P
1	C	1034	PTR	CZ-OH-P-O2P

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	1034	PTR	2	0
1	A	1035	PTR	1	0
1	C	1034	PTR	2	0
1	B	1034	PTR	3	0
1	C	1035	PTR	3	0
1	A	1034	PTR	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	C	1202	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	A	1203	-	3,3,3	0.41	0	2,2,2	0.40	0
3	EDO	C	1205	-	3,3,3	0.43	0	2,2,2	0.26	0
3	EDO	D	1202	-	3,3,3	0.42	0	2,2,2	0.41	0
3	EDO	A	1204	-	3,3,3	0.42	0	2,2,2	0.60	0
3	EDO	B	1202	-	3,3,3	0.37	0	2,2,2	0.54	0
3	EDO	D	1203	-	3,3,3	0.49	0	2,2,2	0.26	0
2	JAK	A	1201	-	15,22,22	1.21	3 (20%)	16,32,32	3.29	5 (31%)
2	JAK	D	1201	-	15,22,22	1.08	0	16,32,32	2.99	5 (31%)
3	EDO	A	1202	-	3,3,3	0.43	0	2,2,2	0.42	0
3	EDO	A	1206	-	3,3,3	0.42	0	2,2,2	0.46	0
3	EDO	C	1203	-	3,3,3	0.53	0	2,2,2	0.32	0
3	EDO	C	1204	-	3,3,3	0.41	0	2,2,2	0.42	0
3	EDO	A	1205	-	3,3,3	0.44	0	2,2,2	0.54	0
2	JAK	C	1201	-	15,22,22	1.23	2 (13%)	16,32,32	3.01	6 (37%)
2	JAK	B	1201	-	15,22,22	1.17	1 (6%)	16,32,32	3.04	5 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	1202	-	-	0/1/1/1	-
3	EDO	A	1203	-	-	0/1/1/1	-
3	EDO	C	1205	-	-	0/1/1/1	-
3	EDO	D	1202	-	-	0/1/1/1	-
3	EDO	A	1204	-	-	1/1/1/1	-
3	EDO	B	1202	-	-	1/1/1/1	-
3	EDO	D	1203	-	-	1/1/1/1	-
2	JAK	A	1201	-	-	0/0/12/12	0/4/4/4
2	JAK	D	1201	-	-	0/0/12/12	0/4/4/4
3	EDO	A	1202	-	-	0/1/1/1	-
3	EDO	A	1206	-	-	0/1/1/1	-
3	EDO	C	1203	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	1204	-	-	1/1/1/1	-
3	EDO	A	1205	-	-	1/1/1/1	-
2	JAK	C	1201	-	-	0/0/12/12	0/4/4/4
2	JAK	B	1201	-	-	0/0/12/12	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	JAK	C7-N6	-3.13	1.32	1.37
2	B	1201	JAK	C7-N6	-2.95	1.33	1.37
2	A	1201	JAK	C2-N3	-2.51	1.29	1.34
2	A	1201	JAK	C7-N6	-2.25	1.34	1.37
2	A	1201	JAK	C7-N19	2.23	1.38	1.34
2	C	1201	JAK	C2-N3	-2.15	1.30	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	JAK	C5-N6-C7	9.53	123.19	117.40
2	B	1201	JAK	C5-N6-C7	9.04	122.89	117.40
2	D	1201	JAK	C5-N6-C7	8.00	122.26	117.40
2	C	1201	JAK	C5-N6-C7	7.97	122.24	117.40
2	A	1201	JAK	C8-C9-C4	-6.52	116.54	120.03
2	C	1201	JAK	C8-C9-C4	-5.92	116.86	120.03
2	D	1201	JAK	C8-C9-C4	-5.49	117.09	120.03
2	B	1201	JAK	C8-C9-C4	-4.98	117.36	120.03
2	D	1201	JAK	C15-C16-C11	-4.37	107.02	110.44
2	A	1201	JAK	C8-C9-N10	4.06	138.23	130.91
2	C	1201	JAK	C2-N10-C11	-3.86	122.40	125.50
2	C	1201	JAK	C8-C9-N10	3.65	137.50	130.91
2	D	1201	JAK	C2-N10-C11	-3.65	122.57	125.50
2	B	1201	JAK	C8-C9-N10	3.63	137.47	130.91
2	D	1201	JAK	C8-C9-N10	3.52	137.25	130.91
2	B	1201	JAK	C15-C16-C11	-3.50	107.70	110.44
2	A	1201	JAK	C2-N10-C11	-3.24	122.90	125.50
2	C	1201	JAK	C15-C16-C11	-2.80	108.25	110.44
2	A	1201	JAK	C15-C16-C11	-2.60	108.41	110.44
2	B	1201	JAK	C2-N10-C11	-2.57	123.43	125.50
2	C	1201	JAK	C13-C12-C11	-2.46	108.52	110.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	EDO	O1-C1-C2-O2
3	B	1202	EDO	O1-C1-C2-O2
3	D	1203	EDO	O1-C1-C2-O2
3	A	1205	EDO	O1-C1-C2-O2
3	C	1203	EDO	O1-C1-C2-O2
3	C	1204	EDO	O1-C1-C2-O2

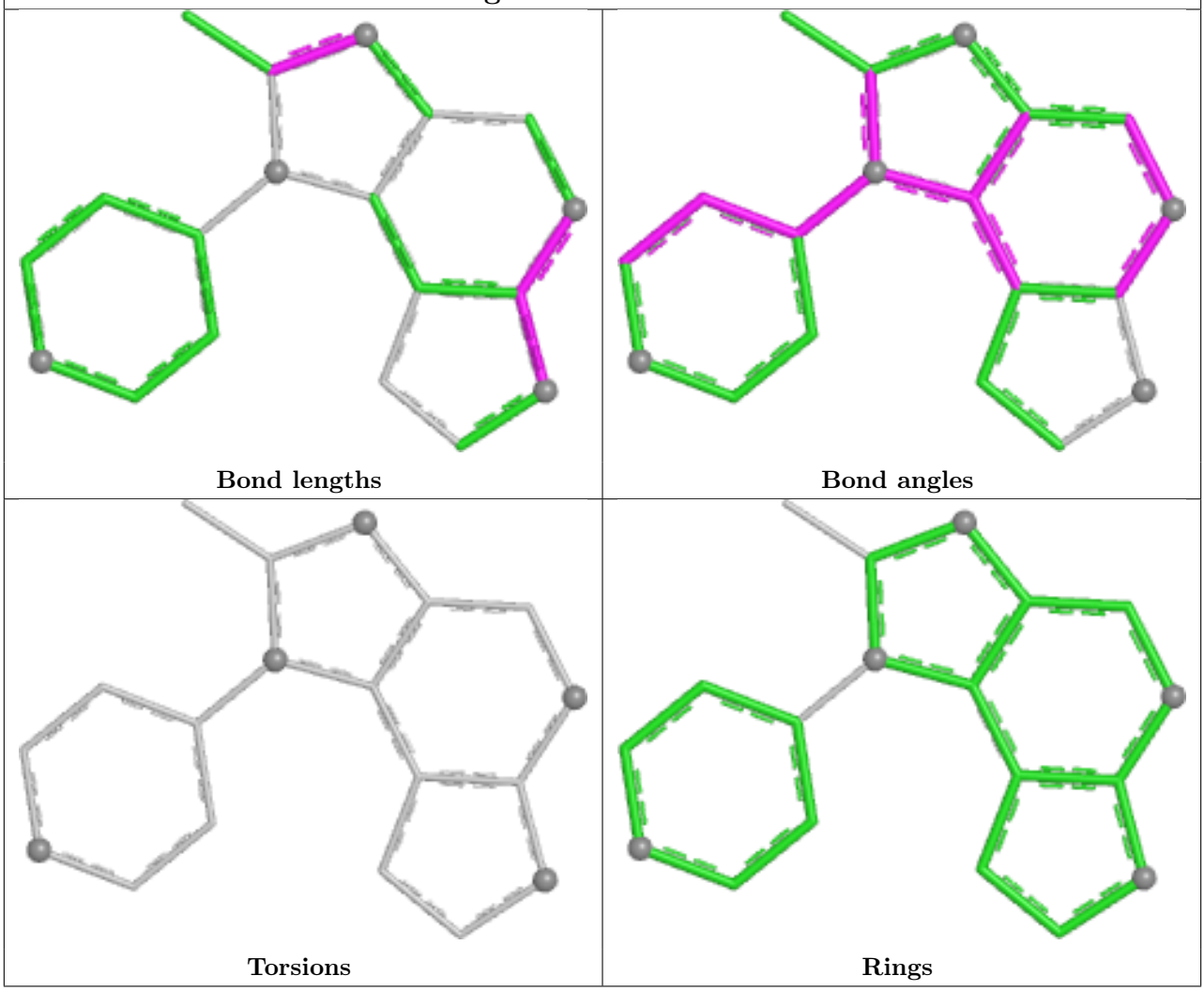
There are no ring outliers.

10 monomers are involved in 21 short contacts:

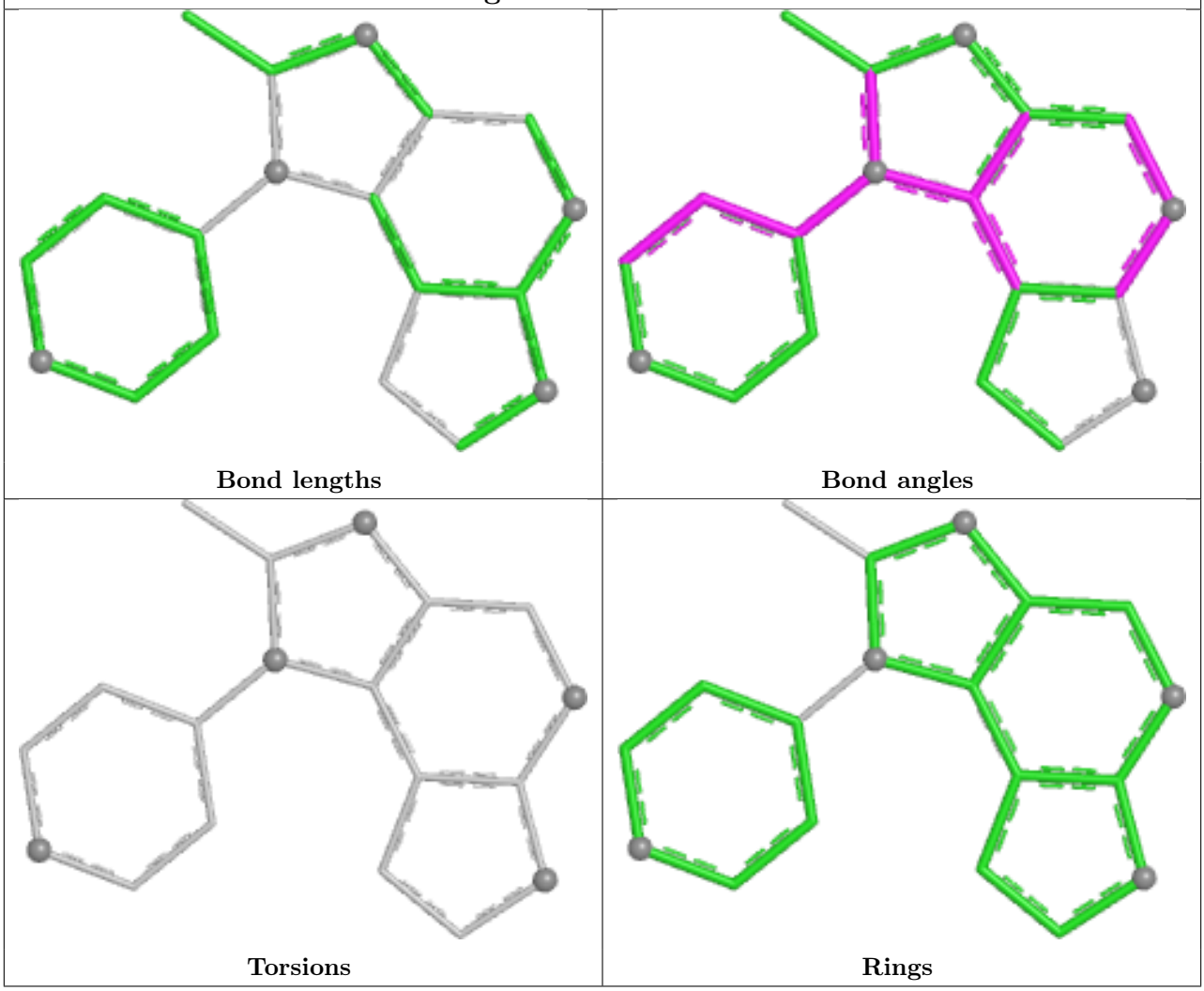
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1202	EDO	2	0
3	A	1203	EDO	1	0
3	C	1205	EDO	7	0
3	D	1203	EDO	5	0
2	D	1201	JAK	1	0
3	A	1202	EDO	1	0
3	A	1206	EDO	1	0
3	C	1203	EDO	1	0
2	C	1201	JAK	1	0
2	B	1201	JAK	1	0

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

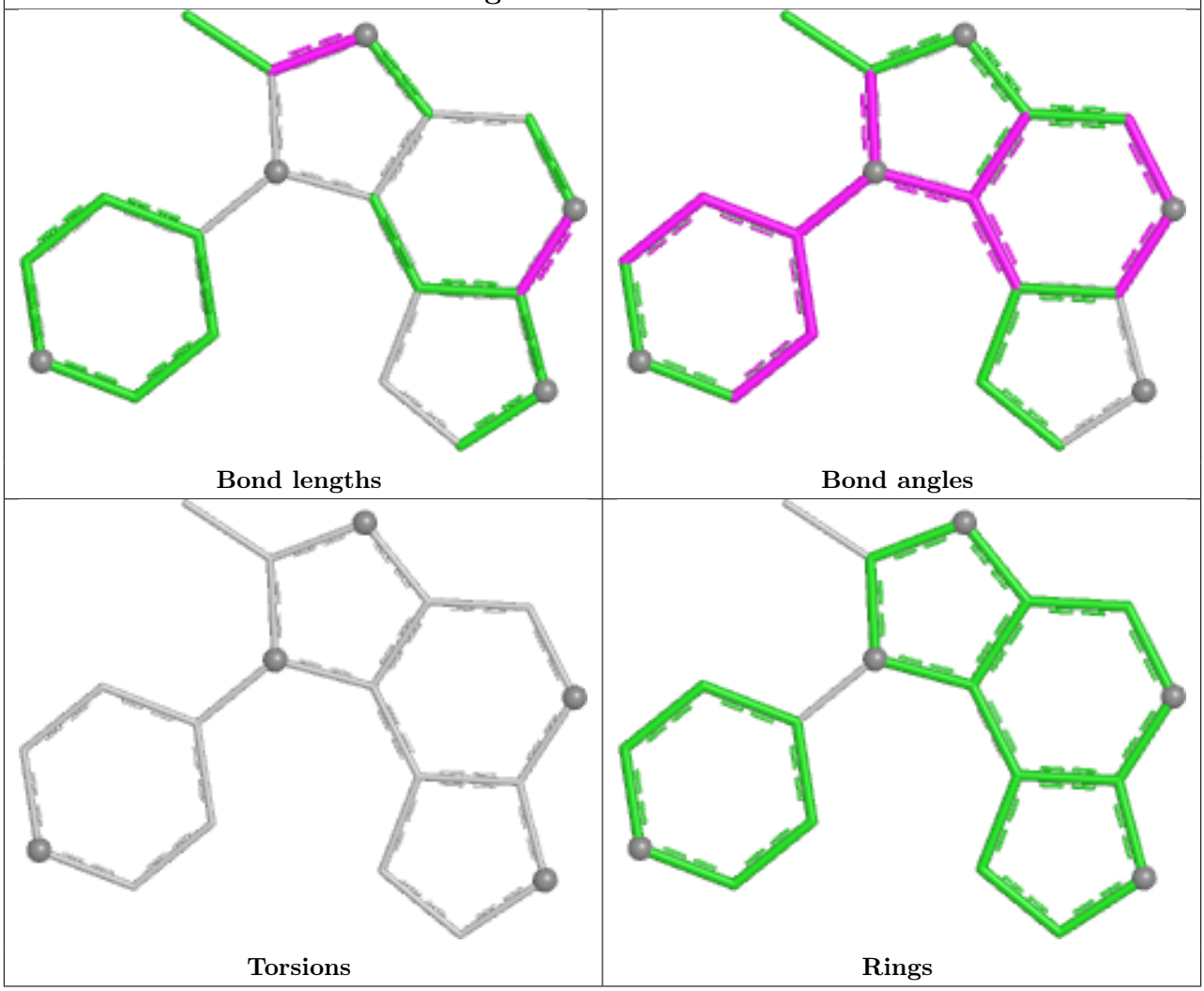
Ligand JAK A 1201



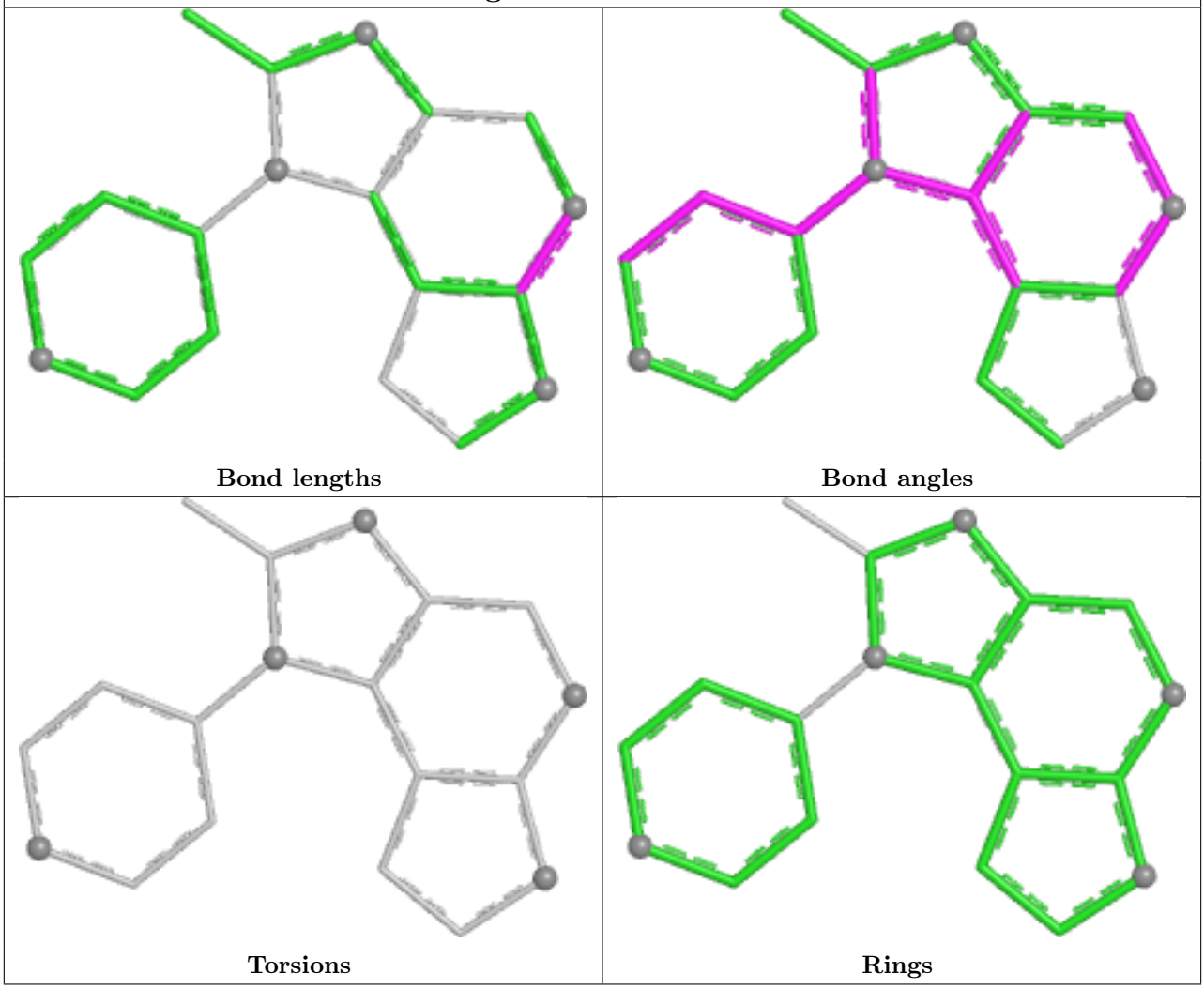
Ligand JAK D 1201



Ligand JAK C 1201



Ligand JAK B 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	290/302 (96%)	-0.18	13 (4%)	33	34	12, 27, 61, 102	0
1	B	280/302 (92%)	-0.22	6 (2%)	63	64	12, 28, 57, 89	0
1	C	278/302 (92%)	-0.30	6 (2%)	62	62	11, 24, 52, 90	0
1	D	280/302 (92%)	-0.18	7 (2%)	57	58	11, 27, 59, 88	0
All	All	1128/1208 (93%)	-0.22	32 (2%)	53	54	11, 27, 58, 102	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	861	PRO	5.5
1	A	863	THR	5.1
1	C	885	HIS	4.7
1	A	862	ALA	4.6
1	B	1030	THR	4.4
1	A	1031	ASP	4.3
1	A	859	LYS	3.8
1	A	885	HIS	3.6
1	A	860	LYS	3.6
1	A	1030	THR	3.4
1	C	886	PHE	3.3
1	B	885	HIS	3.3
1	B	1031	ASP	3.1
1	D	885	HIS	3.1
1	D	1031	ASP	3.1
1	B	950	ASN	3.0
1	D	950	ASN	3.0
1	D	1154	LYS	2.9
1	B	865	VAL	2.8
1	D	865	VAL	2.8
1	C	912	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	947	ASP	2.7
1	D	886	PHE	2.6
1	A	1095	THR	2.6
1	D	1030	THR	2.5
1	C	884	GLY	2.5
1	B	1029	GLU	2.5
1	C	1095	THR	2.4
1	C	1031	ASP	2.4
1	A	912	PRO	2.2
1	A	1154	LYS	2.1
1	A	950	ASN	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	PTR	C	1034	16/17	0.88	0.17	26,43,66,67	0
1	PTR	B	1035	16/17	0.89	0.12	26,41,60,66	0
1	PTR	A	1034	16/17	0.89	0.14	25,47,65,75	0
1	PTR	A	1035	16/17	0.90	0.13	29,54,69,79	0
1	PTR	D	1034	16/17	0.91	0.14	21,49,82,84	0
1	PTR	C	1035	16/17	0.92	0.12	25,35,65,68	0
1	PTR	B	1034	16/17	0.93	0.13	31,54,73,77	0
1	PTR	D	1035	16/17	0.93	0.10	24,37,55,57	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

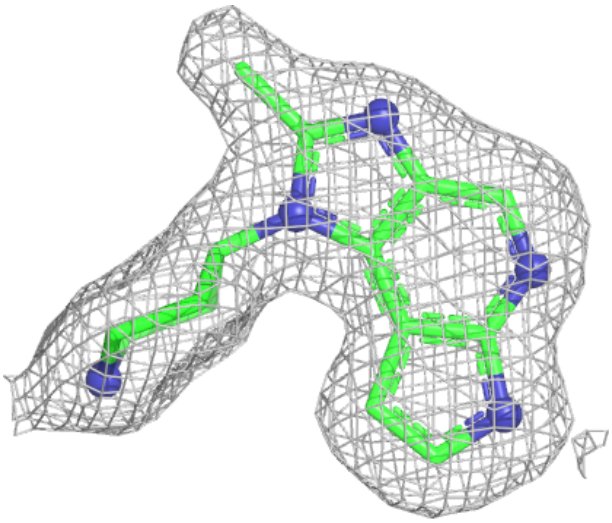
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

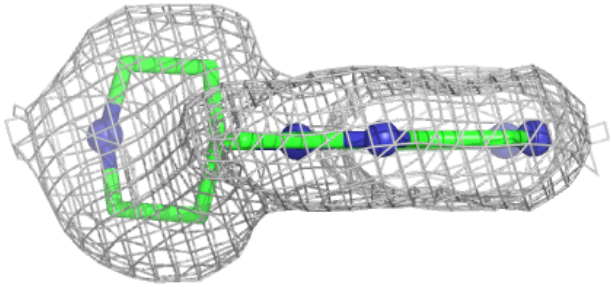
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	1203	4/4	0.81	0.15	44,50,54,54	0
3	EDO	B	1202	4/4	0.83	0.21	49,50,51,57	0
3	EDO	C	1204	4/4	0.84	0.17	38,39,44,49	0
3	EDO	D	1203	4/4	0.86	0.35	34,37,42,54	0
3	EDO	A	1204	4/4	0.91	0.18	41,46,48,49	0
3	EDO	C	1205	4/4	0.93	0.16	50,54,60,62	0
3	EDO	A	1203	4/4	0.93	0.14	40,46,46,47	0
3	EDO	C	1202	4/4	0.94	0.27	36,49,51,53	0
3	EDO	A	1205	4/4	0.96	0.12	43,45,52,56	0
3	EDO	D	1202	4/4	0.96	0.21	20,30,40,48	0
3	EDO	A	1206	4/4	0.96	0.24	43,48,52,55	0
3	EDO	A	1202	4/4	0.97	0.08	22,22,35,44	0
2	JAK	A	1201	19/19	0.97	0.10	7,12,22,23	0
2	JAK	C	1201	19/19	0.97	0.08	8,13,18,19	0
2	JAK	B	1201	19/19	0.98	0.07	9,14,21,23	0
2	JAK	D	1201	19/19	0.98	0.09	9,12,16,18	0

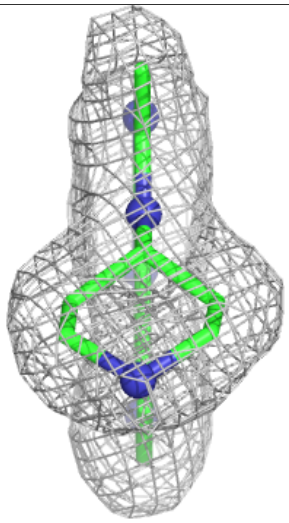
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JAK 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)

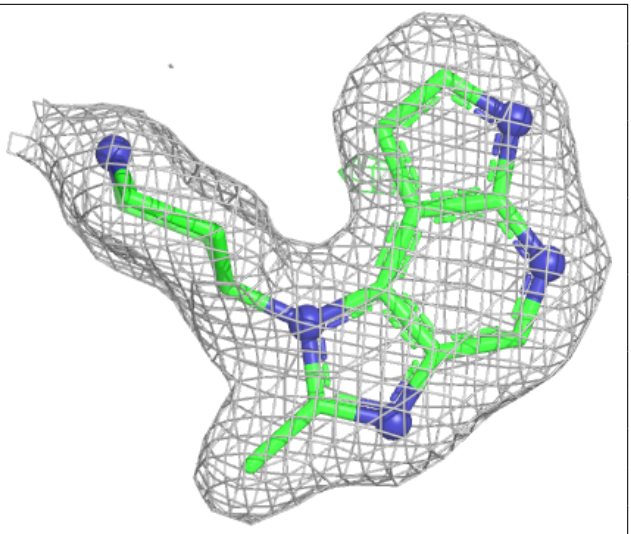


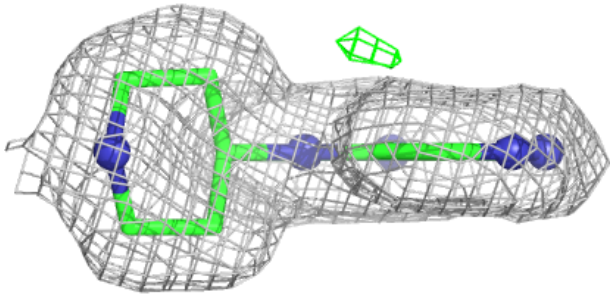


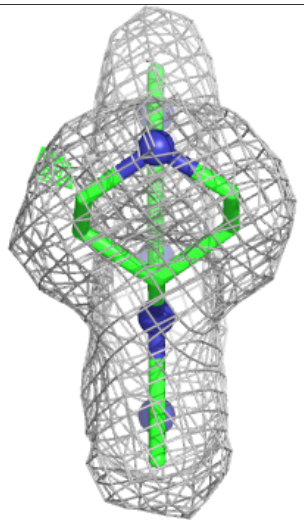


Electron density around JAK C 1201:

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

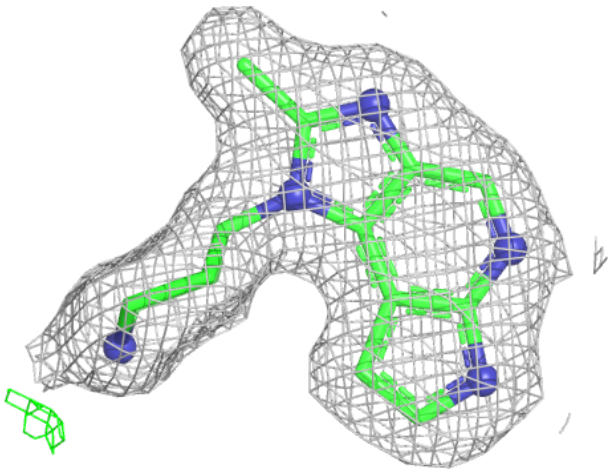


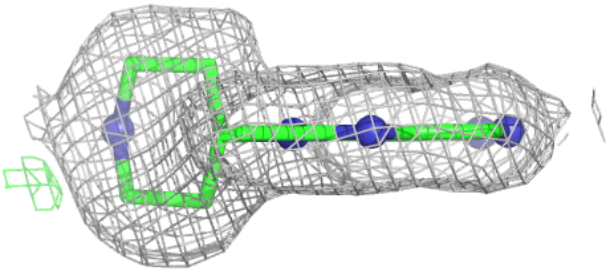


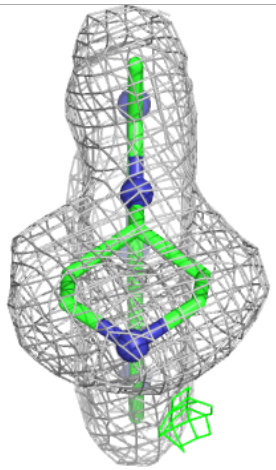


Electron density around JAK B 1201:

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

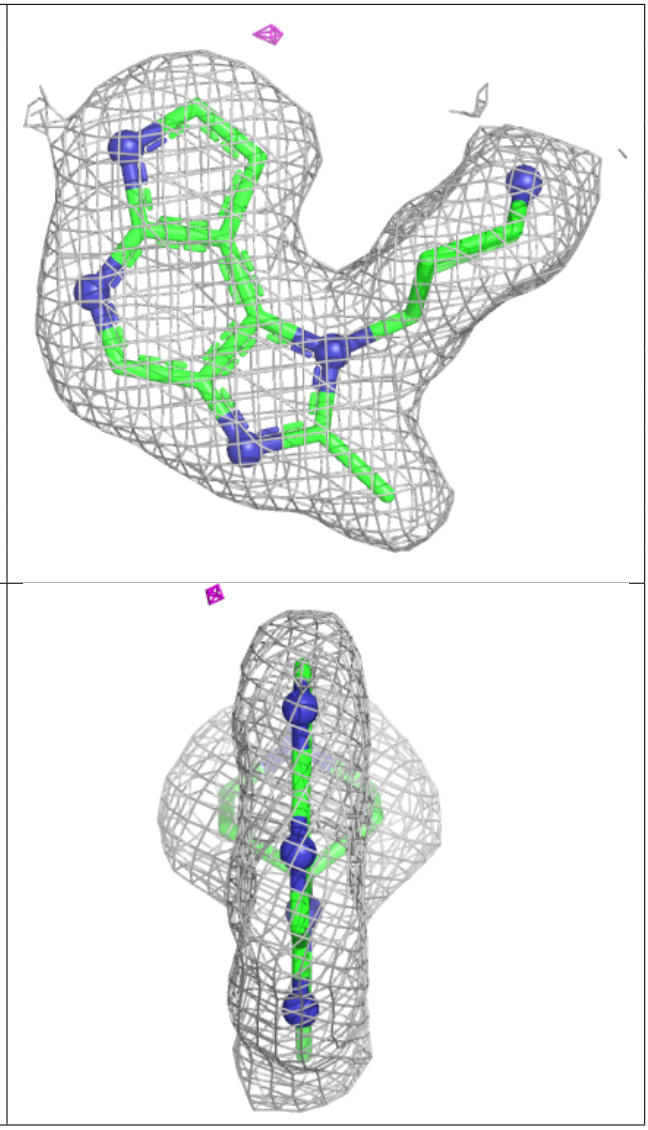






Electron density around JAK D 1201:

$2mF_o$-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.