



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:20 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

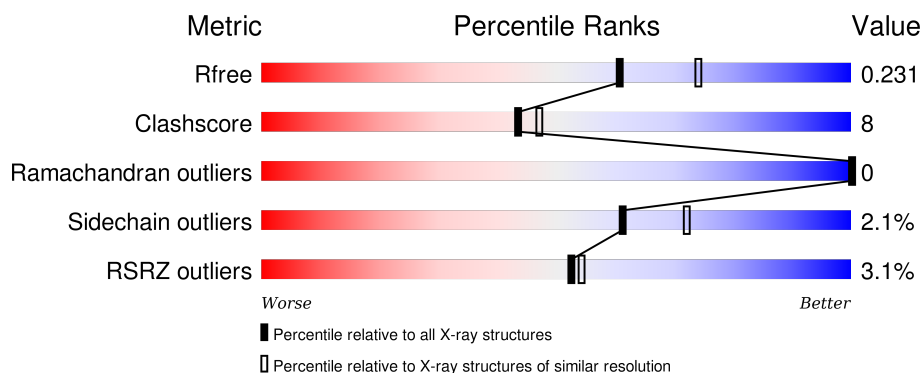
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>5%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	B	302	<div> <div>2%</div> <div>80%</div> <div>12%</div> <div>• 7%</div> </div>
1	C	302	<div> <div>2%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>
1	D	302	<div> <div>3%</div> <div>78%</div> <div>15%</div> <div>• 7%</div> </div>

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	A	1203	-	-	-	X
3	EDO	A	1204	-	-	-	X
3	EDO	A	1206	-	-	-	X
3	EDO	B	1202	-	-	-	X
3	EDO	C	1202	-	-	-	X
3	EDO	C	1204	-	-	-	X
3	EDO	C	1205	-	-	X	-
3	EDO	D	1202	-	-	-	X
3	EDO	D	1203	-	-	X	X

## 2 Entry composition

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.

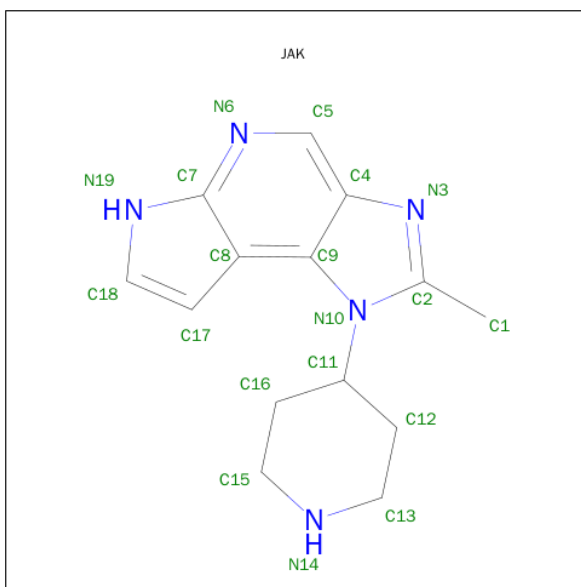
- Molecule 1 is a protein called Tyrosine-protein kinase JAK1.

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

There are 4 discrepancies between the modelled and reference sequences:

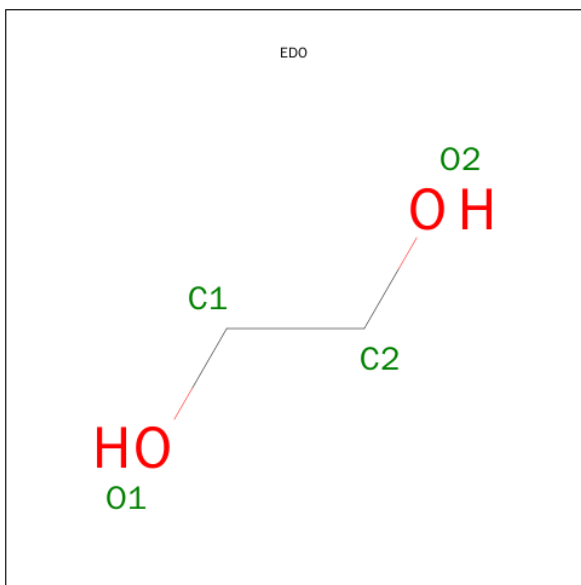
Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	-	EXPRESSION TAG	UNP P23458
B	853	GLY	-	EXPRESSION TAG	UNP P23458
C	853	GLY	-	EXPRESSION TAG	UNP P23458
D	853	GLY	-	EXPRESSION TAG	UNP P23458

- 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<sub>14</sub>H<sub>17</sub>N<sub>5</sub>).



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

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



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

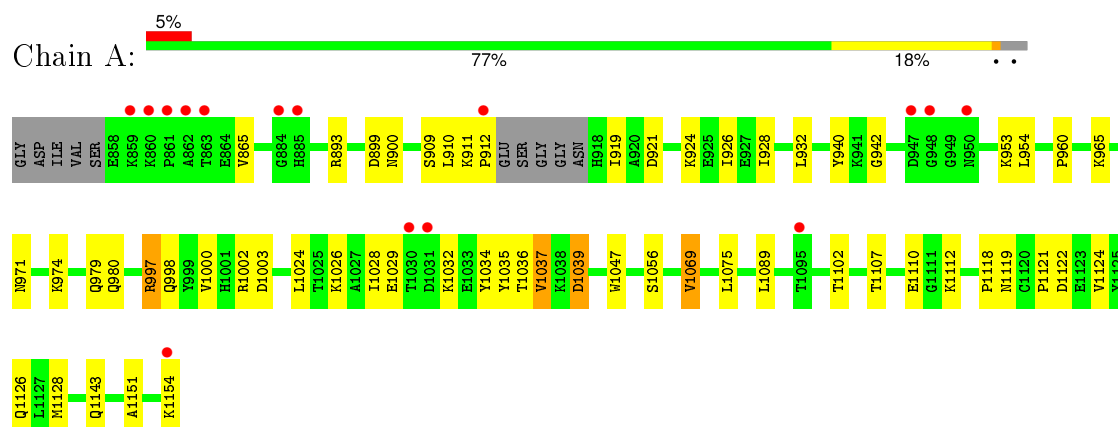
- Molecule 4 is water.

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

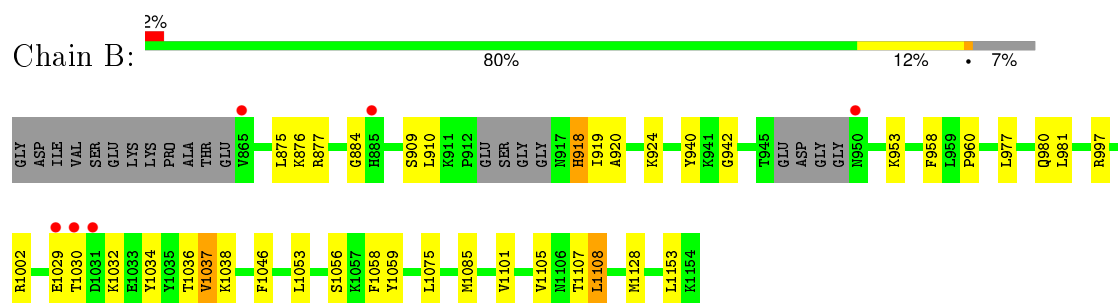
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

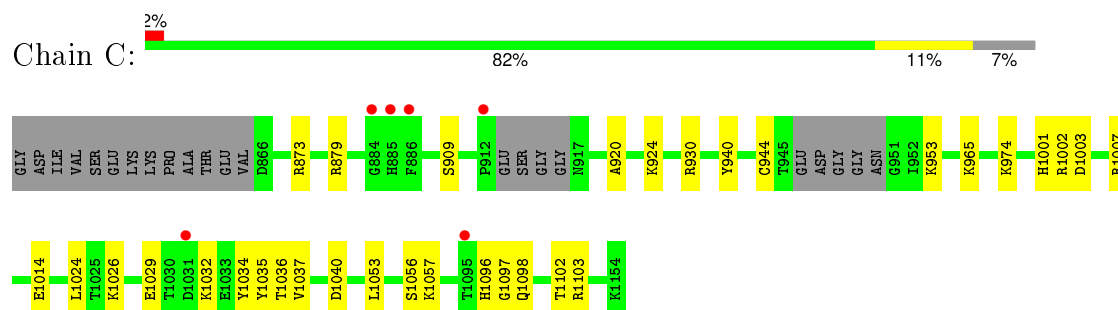
- Molecule 1: Tyrosine-protein kinase JAK1



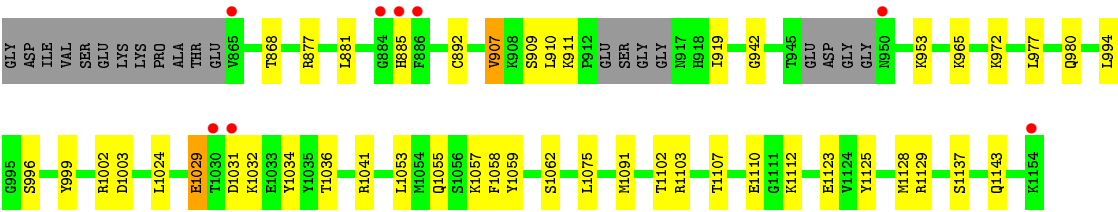
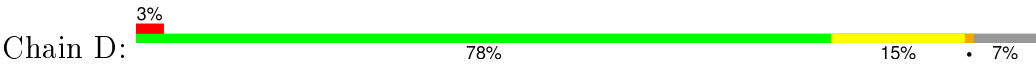
- Molecule 1: Tyrosine-protein kinase JAK1



- Molecule 1: Tyrosine-protein kinase JAK1



- Molecule 1: Tyrosine-protein kinase JAK1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_648)	Depositor
R, $R_{free}$	0.171 , 0.229 0.177 , 0.231	Depositor DCC
$R_{free}$ test set	3211 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.7	EDS
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 63564 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PTR, EDO, JAK

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:C:1040:ASP:HB3	3:C:1205:EDO:H11	1.81	0.62
1:B:920:ALA:O	1:B:924:LYS:HE2	1.98	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:C	1:A:1039:ASP:OD1	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:C:1026:LYS:HG2	1:C:1035:PTR:CZ	2.40	0.52
1:A:980:GLN:HE22	3:A:1203:EDO:H12	1.75	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:HD3	1:B:924:LYS:N	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:C:1002:ARG:NH1	1:C:1026:LYS:HD3	2.28	0.48
1:A:1039:ASP:OD1	1:A:1039:ASP:O	2.31	0.48
1:B:1034:PTR:HD1	1:B:1059:TYR:CE2	2.49	0.48
1:C:1026:LYS:HG2	1:C:1035:PTR:CE1	2.43	0.48
1:A:1110:GLU:HB3	1:A:1112:LYS:HZ3	1.78	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:1029:GLU:CD	1:B:1029:GLU:H	2.16	0.47
1:B:940:TYR:CZ	1:B:942:GLY:HA2	2.50	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:B:920:ALA:O	1:B:924:LYS:HG2	2.15	0.46
1:A:893:ARG:NE	1:A:900:ASN:ND2	2.63	0.46
1:A:1003:ASP:HB2	1:A:1024:LEU:HD12	1.96	0.46
1:A:909:SER:HB3	1:A:953:LYS:HG2	1.97	0.46
1:B:1037:VAL:HG13	1:B:1056:SER:O	2.15	0.46
1:A:940:TYR:CZ	1:A:942:GLY:HA2	2.50	0.46
1:B:977:LEU:HA	1:B:980:GLN:OE1	2.17	0.45
2:B:1201:JAK:H11	2:B:1201:JAK:H1	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:H11	2:D:1201:JAK:H1	1.84	0.45
1:A:910:LEU:HD11	1:A:919:ILE:HA	1.99	0.45
1:D:972:LYS:N	3:D:1203:EDO:C1	2.75	0.44
1:C:1096:HIS:CD2	1:C:1103:ARG:HG3	2.53	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:HB3	1:D:1057:LYS:HE2	1.85	0.43
1:A:1034:PTR:HE2	1:A:1036:THR:OG1	2.19	0.43
1:D:885:HIS:C	1:D:911:LYS:HE3	2.38	0.43
1:A:997:ARG:O	1:A:998:GLN:HB2	2.19	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:C	1:B:1034:PTR:HD2	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:C:1034:PTR:HE1	1:C:1034:PTR:O3P	2.20	0.42
1:B:877:ARG:NH2	1:D:1137:SER:O	2.52	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:D:1059:TYR:CD1	1:D:1059:TYR:N	2.88	0.41
1:D:1003:ASP:HB2	1:D:1024:LEU:HD12	2.02	0.41
1:A:1121:PRO:HG2	1:A:1124:VAL:HG23	2.01	0.41
1:A:1075:LEU:HD12	1:A:1128:MET:HE1	2.02	0.41
1:B:918:HIS:N	1:B:918:HIS:ND1	2.67	0.41
1:A:1075:LEU:HD12	1:A:1128:MET:CE	2.51	0.41
1:A:1089:LEU:HA	1:A:1089:LEU:HD23	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%)	52	62
1	B	254/267 (95%)	248 (98%)	6 (2%)	57	67
1	C	251/267 (94%)	249 (99%)	2 (1%)	86	93
1	D	253/267 (95%)	247 (98%)	6 (2%)	57	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1016/1068 (95%)	995 (98%)	21 (2%)	61	72

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

Some 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 ⓘ

There are no RNA molecules in this entry.



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

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	A	1034	1	14,16,17	1.86	1 (7%)	18,22,24	0.94	1 (5%)
1	PTR	A	1035	1	14,16,17	1.74	1 (7%)	18,22,24	0.78	1 (5%)
1	PTR	B	1034	1	14,16,17	1.90	1 (7%)	18,22,24	0.69	0
1	PTR	B	1035	1	14,16,17	1.72	1 (7%)	18,22,24	0.75	0
1	PTR	C	1034	1	14,16,17	1.86	1 (7%)	18,22,24	0.85	1 (5%)
1	PTR	C	1035	1	14,16,17	1.78	1 (7%)	18,22,24	0.82	1 (5%)
1	PTR	D	1034	1	14,16,17	1.80	1 (7%)	18,22,24	0.79	0
1	PTR	D	1035	1	14,16,17	1.82	1 (7%)	18,22,24	0.72	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	A	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1035	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1035	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1035	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1035	1	-	0/9/11/13	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	-7.00	1.23	1.40
1	C	1034	PTR	OH-CZ	-6.77	1.24	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1034	PTR	OH-CZ	-6.74	1.24	1.40
1	D	1035	PTR	OH-CZ	-6.62	1.24	1.40
1	D	1034	PTR	OH-CZ	-6.59	1.24	1.40
1	C	1035	PTR	OH-CZ	-6.49	1.25	1.40
1	A	1035	PTR	OH-CZ	-6.33	1.25	1.40
1	B	1035	PTR	OH-CZ	-6.22	1.25	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1035	PTR	O-C-CA	-2.22	119.70	125.49
1	A	1034	PTR	O-C-CA	-2.07	120.11	125.49
1	A	1035	PTR	O-C-CA	-2.02	120.22	125.49
1	C	1034	PTR	O3P-P-OH	2.21	113.16	105.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
2	JAK	A	1201	-	15,22,22	4.94	7 (46%)	15,32,32	3.13	6 (40%)
3	EDO	A	1202	-	3,3,3	0.48	0	2,2,2	0.47	0
3	EDO	A	1203	-	3,3,3	0.45	0	2,2,2	0.44	0
3	EDO	A	1204	-	3,3,3	0.46	0	2,2,2	0.66	0
3	EDO	A	1205	-	3,3,3	0.48	0	2,2,2	0.60	0
3	EDO	A	1206	-	3,3,3	0.47	0	2,2,2	0.51	0
2	JAK	B	1201	-	15,22,22	4.80	7 (46%)	15,32,32	2.94	7 (46%)
3	EDO	B	1202	-	3,3,3	0.41	0	2,2,2	0.59	0
2	JAK	C	1201	-	15,22,22	4.84	7 (46%)	15,32,32	2.93	6 (40%)
3	EDO	C	1202	-	3,3,3	0.49	0	2,2,2	0.41	0
3	EDO	C	1203	-	3,3,3	0.57	0	2,2,2	0.36	0
3	EDO	C	1204	-	3,3,3	0.45	0	2,2,2	0.46	0
3	EDO	C	1205	-	3,3,3	0.47	0	2,2,2	0.30	0
2	JAK	D	1201	-	15,22,22	4.75	7 (46%)	15,32,32	3.00	7 (46%)
3	EDO	D	1202	-	3,3,3	0.46	0	2,2,2	0.46	0
3	EDO	D	1203	-	3,3,3	0.52	0	2,2,2	0.30	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
2	JAK	A	1201	-	-	0/4/12/12	0/4/4/4
3	EDO	A	1202	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1203	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1204	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1205	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1206	-	-	0/1/1/1	0/0/0/0
2	JAK	B	1201	-	-	0/4/12/12	0/4/4/4
3	EDO	B	1202	-	-	0/1/1/1	0/0/0/0
2	JAK	C	1201	-	-	0/4/12/12	0/4/4/4
3	EDO	C	1202	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1203	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1204	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1205	-	-	0/1/1/1	0/0/0/0
2	JAK	D	1201	-	-	0/4/12/12	0/4/4/4
3	EDO	D	1202	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	1203	-	-	0/1/1/1	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	JAK	C5-N6	-10.02	1.30	1.47
2	B	1201	JAK	C5-N6	-9.59	1.31	1.47
2	C	1201	JAK	C5-N6	-9.24	1.32	1.47
2	D	1201	JAK	C8-C9	-9.08	1.41	1.54
2	B	1201	JAK	C8-C9	-8.97	1.41	1.54
2	D	1201	JAK	C5-N6	-8.90	1.32	1.47
2	C	1201	JAK	C8-C9	-8.89	1.41	1.54
2	A	1201	JAK	C4-N3	-8.63	1.34	1.48
2	A	1201	JAK	C8-C9	-8.61	1.41	1.54
2	D	1201	JAK	C4-N3	-8.26	1.35	1.48
2	C	1201	JAK	C4-N3	-8.17	1.35	1.48
2	B	1201	JAK	C4-N3	-8.08	1.35	1.48
2	A	1201	JAK	C2-N10	-8.01	1.37	1.47
2	C	1201	JAK	C2-N10	-7.93	1.37	1.47
2	D	1201	JAK	C2-N10	-7.79	1.37	1.47
2	B	1201	JAK	C2-N10	-7.27	1.38	1.47
2	C	1201	JAK	C9-N10	-6.24	1.38	1.48
2	B	1201	JAK	C9-N10	-6.12	1.38	1.48
2	A	1201	JAK	C9-N10	-5.82	1.39	1.48
2	D	1201	JAK	C9-N10	-5.62	1.39	1.48
2	A	1201	JAK	C18-N19	-3.36	1.36	1.48
2	C	1201	JAK	C18-N19	-3.32	1.37	1.48
2	B	1201	JAK	C18-N19	-3.24	1.37	1.48
2	D	1201	JAK	C18-N19	-3.10	1.37	1.48
2	C	1201	JAK	C17-C8	-2.66	1.46	1.54
2	A	1201	JAK	C17-C8	-2.48	1.47	1.54
2	B	1201	JAK	C17-C8	-2.41	1.47	1.54
2	D	1201	JAK	C17-C8	-2.30	1.47	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	JAK	C15-C16-C11	-2.48	107.02	110.80
2	B	1201	JAK	C15-C16-C11	-2.04	107.70	110.80
2	A	1201	JAK	C5-C4-N3	2.76	131.83	117.91
2	D	1201	JAK	C18-C17-C8	2.85	107.37	104.02
2	B	1201	JAK	C18-C17-C8	2.85	107.38	104.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	JAK	C5-C4-N3	2.89	132.50	117.91
2	D	1201	JAK	C5-C4-N3	2.94	132.72	117.91
2	C	1201	JAK	C5-C4-N3	3.02	133.13	117.91
2	C	1201	JAK	C18-C17-C8	3.14	107.72	104.02
2	A	1201	JAK	C18-C17-C8	3.35	107.97	104.02
2	A	1201	JAK	C18-N19-C7	3.42	109.30	105.40
2	B	1201	JAK	C18-N19-C7	3.56	109.46	105.40
2	D	1201	JAK	C9-C4-N3	3.98	107.06	102.13
2	A	1201	JAK	C9-C4-N3	4.19	107.32	102.13
2	C	1201	JAK	C9-C4-N3	4.20	107.33	102.13
2	C	1201	JAK	C18-N19-C7	4.24	110.24	105.40
2	D	1201	JAK	C18-N19-C7	4.32	110.33	105.40
2	B	1201	JAK	C5-C4-C9	4.53	119.28	111.15
2	C	1201	JAK	C5-C4-C9	4.68	119.54	111.15
2	B	1201	JAK	C9-C4-N3	4.91	108.22	102.13
2	D	1201	JAK	C5-C4-C9	5.06	120.22	111.15
2	A	1201	JAK	C5-C4-C9	5.41	120.86	111.15
2	C	1201	JAK	C1-C2-N10	6.61	124.76	112.92
2	B	1201	JAK	C1-C2-N10	6.69	124.90	112.92
2	D	1201	JAK	C1-C2-N10	6.86	125.20	112.92
2	A	1201	JAK	C1-C2-N10	7.66	126.64	112.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 21 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	290/302 (96%)	-0.13	15 (5%) 31 33	12, 27, 61, 102	0
1	B	280/302 (92%)	-0.18	6 (2%) 67 68	12, 28, 57, 89	0
1	C	278/302 (92%)	-0.26	6 (2%) 65 66	11, 24, 52, 90	0
1	D	280/302 (92%)	-0.13	8 (2%) 55 57	11, 27, 59, 88	0
All	All	1128/1208 (93%)	-0.17	35 (3%) 52 54	11, 27, 58, 102	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	861	PRO	5.7
1	A	863	THR	5.3
1	C	885	HIS	4.9
1	A	862	ALA	4.9
1	B	1030	THR	4.6
1	A	1031	ASP	4.5
1	A	859	LYS	3.9
1	A	885	HIS	3.8
1	A	860	LYS	3.7
1	A	1030	THR	3.6
1	C	886	PHE	3.5
1	B	885	HIS	3.4
1	B	1031	ASP	3.3
1	D	1031	ASP	3.2
1	D	885	HIS	3.2
1	B	865	VAL	3.1
1	B	950	ASN	3.1
1	D	865	VAL	3.1
1	D	950	ASN	3.1
1	D	1154	LYS	3.0
1	D	886	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	912	PRO	2.8
1	A	947	ASP	2.8
1	A	1095	THR	2.8
1	C	884	GLY	2.6
1	C	1095	THR	2.6
1	D	1030	THR	2.6
1	C	1031	ASP	2.6
1	B	1029	GLU	2.5
1	A	912	PRO	2.2
1	A	1154	LYS	2.2
1	A	950	ASN	2.2
1	A	884	GLY	2.1
1	A	948	GLY	2.1
1	D	884	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PTR	B	1035	16/17	0.89	0.12	-	26,41,60,66	0
1	PTR	D	1035	16/17	0.93	0.10	-	24,37,55,57	0
1	PTR	B	1034	16/17	0.93	0.13	-	31,54,73,77	0
1	PTR	A	1034	16/17	0.89	0.14	-	25,47,65,75	0
1	PTR	C	1034	16/17	0.88	0.17	-	26,43,66,67	0
1	PTR	C	1035	16/17	0.93	0.12	-	25,35,65,68	0
1	PTR	D	1034	16/17	0.91	0.14	-	21,49,82,84	0
1	PTR	A	1035	16/17	0.90	0.13	-	29,54,69,79	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	C	1202	4/4	0.94	0.27	14.05	36,49,51,53	0
3	EDO	C	1204	4/4	0.84	0.17	6.69	38,39,44,49	0
3	EDO	A	1206	4/4	0.96	0.24	6.59	43,48,52,55	0
3	EDO	D	1202	4/4	0.96	0.21	6.52	20,30,40,48	0
3	EDO	D	1203	4/4	0.86	0.34	6.11	34,37,42,54	0
3	EDO	A	1203	4/4	0.93	0.14	4.68	40,46,46,47	0
3	EDO	B	1202	4/4	0.83	0.20	3.89	49,50,51,57	0
3	EDO	A	1204	4/4	0.91	0.18	3.13	41,46,48,49	0
3	EDO	C	1205	4/4	0.93	0.16	1.84	50,54,60,62	0
3	EDO	A	1205	4/4	0.96	0.12	1.11	43,45,52,56	0
3	EDO	A	1202	4/4	0.97	0.08	0.31	22,22,35,44	0
2	JAK	A	1201	19/19	0.97	0.10	-0.05	7,12,22,23	0
2	JAK	D	1201	19/19	0.98	0.09	-0.10	9,12,16,18	0
2	JAK	C	1201	19/19	0.97	0.08	-0.63	8,13,18,19	0
2	JAK	B	1201	19/19	0.98	0.07	-0.91	9,14,21,23	0
3	EDO	C	1203	4/4	0.81	0.15	-	44,50,54,54	0

## 6.5 Other polymers

There are no such residues in this entry.