



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:02 PM GMT

PDB ID : 4BBE  
Title : Aminoalkylpyrimidine Inhibitor Complexes with JAK2  
Authors : Li, J.  
Deposited on : 2012-09-21  
Resolution : 1.90 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

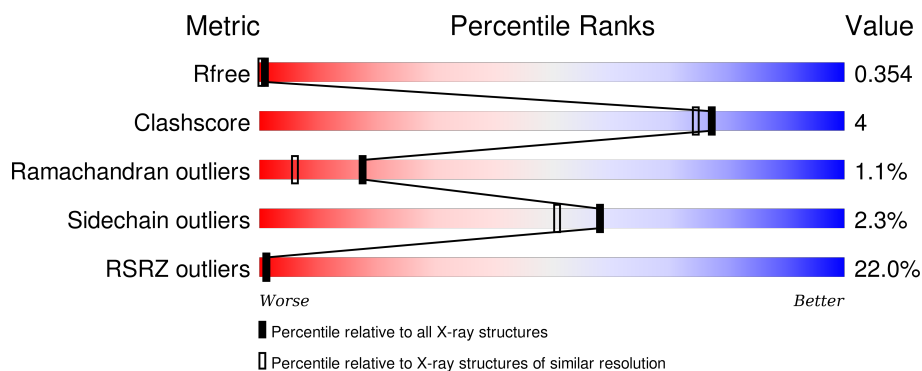
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	298	<div> <div>23%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	B	298	<div> <div>20%</div> <div>88%</div> <div>8%</div> <div>•</div> </div>
1	C	298	<div> <div>19%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	D	298	<div> <div>22%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9717 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.

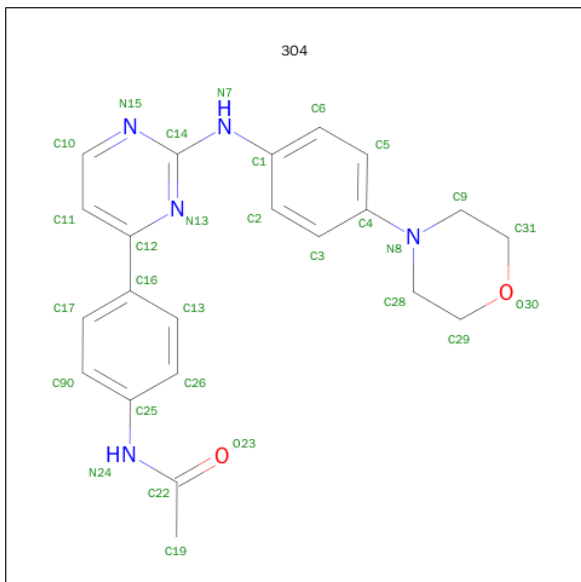
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE JAK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2379	1515	415	436	13			
1	B	288	Total	C	N	O	S	0	0	0
			2379	1515	415	436	13			
1	C	288	Total	C	N	O	S	0	0	0
			2379	1515	415	436	13			
1	D	288	Total	C	N	O	S	0	0	0
			2379	1515	415	436	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	837	GLY	-	EXPRESSION TAG	UNP O60674
A	838	SER	-	EXPRESSION TAG	UNP O60674
A	976	ASN	ASP	ENGINEERED MUTATION	UNP O60674
A	1133	GLU	-	EXPRESSION TAG	UNP O60674
A	1134	PHE	-	EXPRESSION TAG	UNP O60674
B	837	GLY	-	EXPRESSION TAG	UNP O60674
B	838	SER	-	EXPRESSION TAG	UNP O60674
B	976	ASN	ASP	ENGINEERED MUTATION	UNP O60674
B	1133	GLU	-	EXPRESSION TAG	UNP O60674
B	1134	PHE	-	EXPRESSION TAG	UNP O60674
C	837	GLY	-	EXPRESSION TAG	UNP O60674
C	838	SER	-	EXPRESSION TAG	UNP O60674
C	976	ASN	ASP	ENGINEERED MUTATION	UNP O60674
C	1133	GLU	-	EXPRESSION TAG	UNP O60674
C	1134	PHE	-	EXPRESSION TAG	UNP O60674
D	837	GLY	-	EXPRESSION TAG	UNP O60674
D	838	SER	-	EXPRESSION TAG	UNP O60674
D	976	ASN	ASP	ENGINEERED MUTATION	UNP O60674
D	1133	GLU	-	EXPRESSION TAG	UNP O60674
D	1134	PHE	-	EXPRESSION TAG	UNP O60674

- Molecule 2 is N-[4-[2-[(4-MORPHOLIN-4-YL)PHENYL]AMINO]PYRIMIDIN-4-YL]PHENYL]ETHANAMIDE (three-letter code: 3O4) (formula:  $C_{22}H_{23}N_5O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	22	5	2		
2	B	1	Total	C	N	O	0	0
			29	22	5	2		
2	C	1	Total	C	N	O	0	0
			29	22	5	2		
2	D	1	Total	C	N	O	0	0
			29	22	5	2		

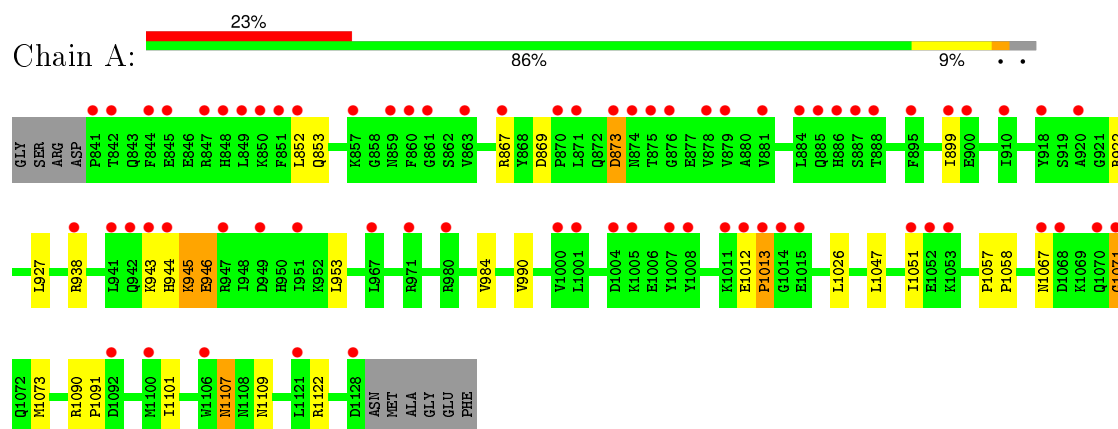
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	18	Total	O	0	0
			18	18		
3	C	28	Total	O	0	0
			28	28		
3	D	17	Total	O	0	0
			17	17		

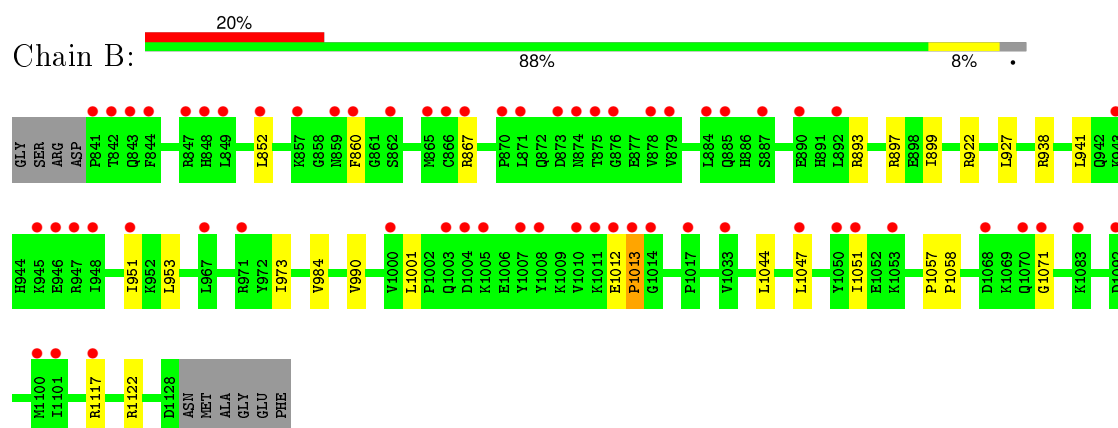
### 3 Residue-property plots

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.

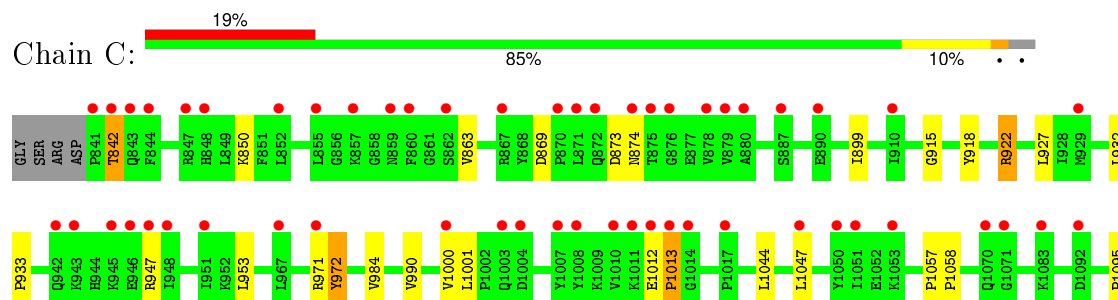
#### • Molecule 1: TYROSINE-PROTEIN KINASE JAK2



#### • Molecule 1: TYROSINE-PROTEIN KINASE JAK2



#### • Molecule 1: TYROSINE-PROTEIN KINASE JAK2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.96Å 76.28Å 87.74Å 84.02° 66.87° 63.13°	Depositor
Resolution (Å)	41.24 – 1.90 41.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (41.24-1.90) 90.8 (41.23-1.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.344 , 0.359 0.339 , 0.354	Depositor DCC
$R_{free}$ test set	5768 reflections (5.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 9.1	EDS
Estimated twinning fraction	0.478 for h,h-k,h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 107635 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 63.07 % 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 1.0234e-05. 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: 3O4

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	0.31	0/2432	0.48	0/3274
1	B	0.31	0/2432	0.46	0/3274
1	C	0.32	0/2432	0.48	0/3274
1	D	0.31	0/2432	0.46	0/3274
All	All	0.31	0/9728	0.47	0/13096

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	2379	0	2369	19	0
1	B	2379	0	2369	12	0
1	C	2379	0	2369	17	0
1	D	2379	0	2369	15	0
2	A	29	0	23	3	0
2	B	29	0	23	4	0
2	C	29	0	23	3	0
2	D	29	0	23	2	0
3	A	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	0	0	0
3	C	28	0	0	0	0
3	D	17	0	0	0	0
All	All	9717	0	9568	70	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 4.

All (70) 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)
2:B:2229:3O4:H2	2:B:2229:3O4:N13	2.00	0.76
1:D:947:ARG:HA	1:D:947:ARG:HH11	1.51	0.75
1:C:971:ARG:N	1:C:972:TYR:HB2	2.05	0.72
1:A:944:HIS:N	1:A:945:LYS:HB2	2.06	0.71
2:D:2229:3O4:N13	2:D:2229:3O4:H2	2.08	0.68
2:A:2229:3O4:N13	2:A:2229:3O4:H6	2.11	0.65
1:A:953:LEU:HD22	1:A:1047:LEU:HB3	1.81	0.63
1:D:947:ARG:HA	1:D:947:ARG:NH1	2.14	0.62
1:D:1012:GLU:N	1:D:1013:PRO:HD2	2.14	0.62
1:C:1012:GLU:N	1:C:1013:PRO:HD2	2.16	0.61
1:A:944:HIS:CA	1:A:945:LYS:HB2	2.31	0.60
1:B:973:ILE:HD11	1:B:1001:LEU:HD13	1.83	0.60
1:C:972:TYR:H	1:C:1000:VAL:HA	1.67	0.60
1:C:918:TYR:HB2	1:C:922:ARG:HD2	1.84	0.59
1:D:1010:VAL:HG12	1:D:1013:PRO:HD3	1.84	0.58
2:C:2229:3O4:N13	2:C:2229:3O4:H2	2.19	0.57
1:C:899:ILE:HG12	1:C:927:LEU:HD13	1.88	0.56
1:D:899:ILE:HG12	1:D:927:LEU:HD13	1.88	0.56
1:A:852:LEU:HD11	1:A:867:ARG:HB2	1.89	0.55
1:B:899:ILE:HG12	1:B:927:LEU:HD13	1.89	0.55
1:A:1012:GLU:N	1:A:1013:PRO:HD2	2.22	0.54
1:B:1012:GLU:N	1:B:1013:PRO:HD2	2.24	0.53
2:B:2229:3O4:N13	2:B:2229:3O4:C2	2.64	0.52
1:A:1101:ILE:HG12	1:A:1122:ARG:HD3	1.91	0.52
1:A:899:ILE:HG12	1:A:927:LEU:HD13	1.91	0.52
2:A:2229:3O4:O23	2:A:2229:3O4:H26	2.10	0.51
1:D:953:LEU:HD22	1:D:1047:LEU:HB3	1.93	0.51
1:D:1012:GLU:N	1:D:1013:PRO:CD	2.73	0.51
1:A:944:HIS:HA	1:A:945:LYS:HB2	1.93	0.51
1:A:1107:ASN:HD22	1:A:1109:ASN:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:LEU:HD12	1:D:983:LEU:HB3	1.94	0.49
1:B:938:ARG:HA	1:B:1051:ILE:HD13	1.94	0.49
2:A:2229:3O4:N13	2:A:2229:3O4:C6	2.74	0.49
1:B:951:ILE:HG12	1:C:947:ARG:HG3	1.95	0.49
1:A:853:GLN:HE22	2:B:2229:3O4:H282	1.79	0.48
1:A:853:GLN:OE1	2:B:2229:3O4:H5	2.14	0.48
1:C:842:THR:O	1:C:915:GLY:HA3	2.14	0.47
1:A:938:ARG:HA	1:A:1051:ILE:HD13	1.96	0.47
1:C:971:ARG:HB3	1:C:1001:LEU:HB2	1.97	0.47
1:C:1044:LEU:HA	1:C:1047:LEU:HD12	1.96	0.47
1:D:1107:ASN:HD22	1:D:1109:ASN:H	1.64	0.46
1:D:932:LEU:HA	1:D:933:PRO:HD3	1.78	0.46
1:A:943:LYS:C	1:A:945:LYS:HB2	2.37	0.46
1:C:1095:PRO:HG2	1:C:1098:ILE:HG12	1.98	0.45
1:B:941:LEU:HD11	1:B:1047:LEU:HD23	1.98	0.45
1:C:953:LEU:HD22	1:C:1047:LEU:HB3	1.98	0.45
1:B:1044:LEU:HA	1:B:1047:LEU:HD12	1.98	0.45
1:C:1107:ASN:HD22	1:C:1109:ASN:H	1.64	0.45
2:D:2229:3O4:C2	2:D:2229:3O4:N13	2.75	0.45
1:D:938:ARG:HA	1:D:1051:ILE:HD13	1.98	0.44
1:D:1062:MET:HA	1:D:1065:ILE:HG12	2.00	0.44
1:C:932:LEU:HA	1:C:933:PRO:HD3	1.78	0.44
1:B:852:LEU:HD11	1:B:867:ARG:HB2	2.00	0.44
1:D:1011:LYS:C	1:D:1013:PRO:HD2	2.38	0.43
1:B:953:LEU:HD22	1:B:1047:LEU:HB3	1.99	0.43
1:C:1057:PRO:HB2	1:C:1058:PRO:HD3	2.00	0.43
1:A:945:LYS:HD3	1:A:946:GLU:HG2	2.01	0.43
1:A:1071:GLY:O	1:A:1073:MET:N	2.44	0.43
1:A:1026:LEU:O	1:D:922:ARG:HD2	2.19	0.42
1:B:1057:PRO:HB2	1:B:1058:PRO:HD3	2.01	0.42
1:D:1057:PRO:HB2	1:D:1058:PRO:HD3	2.02	0.42
1:A:1057:PRO:HB2	1:A:1058:PRO:HD3	2.02	0.42
1:A:984:VAL:HG22	1:A:990:VAL:HG12	2.02	0.41
2:C:2229:3O4:C2	2:C:2229:3O4:N13	2.84	0.41
1:C:1116:PHE:HA	1:C:1119:LEU:HD12	2.02	0.41
1:B:938:ARG:HA	1:B:1051:ILE:CD1	2.50	0.41
1:A:1090:ARG:HA	1:A:1091:PRO:HD3	1.96	0.41
1:C:863:VAL:HG21	2:C:2229:3O4:C25	2.51	0.41
1:B:984:VAL:HG22	1:B:990:VAL:HG12	2.03	0.41
1:C:984:VAL:HG22	1:C:990:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/298 (96%)	264 (92%)	18 (6%)	4 (1%)	14	4
1	B	286/298 (96%)	270 (94%)	14 (5%)	2 (1%)	26	14
1	C	286/298 (96%)	267 (93%)	15 (5%)	4 (1%)	14	4
1	D	286/298 (96%)	269 (94%)	14 (5%)	3 (1%)	19	7
All	All	1144/1192 (96%)	1070 (94%)	61 (5%)	13 (1%)	17	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	945	LYS
1	A	1013	PRO
1	B	1013	PRO
1	C	842	THR
1	C	1013	PRO
1	D	872	GLN
1	A	1071	GLY
1	B	1071	GLY
1	C	873	ASP
1	D	1071	GLY
1	A	873	ASP
1	C	972	TYR
1	D	1013	PRO

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/271 (97%)	257 (98%)	6 (2%)	58	51
1	B	263/271 (97%)	257 (98%)	6 (2%)	58	51
1	C	263/271 (97%)	257 (98%)	6 (2%)	58	51
1	D	263/271 (97%)	257 (98%)	6 (2%)	58	51
All	All	1052/1084 (97%)	1028 (98%)	24 (2%)	58	51

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	869	ASP
1	A	873	ASP
1	A	922	ARG
1	A	946	GLU
1	A	1067	ASN
1	A	1107	ASN
1	B	860	PHE
1	B	893	ARG
1	B	897	ARG
1	B	922	ARG
1	B	1117	ARG
1	B	1122	ARG
1	C	850	LYS
1	C	869	ASP
1	C	874	ASN
1	C	922	ARG
1	C	1107	ASN
1	C	1117	ARG
1	D	873	ASP
1	D	922	ARG
1	D	943	LYS
1	D	947	ARG
1	D	1011	LYS
1	D	1107	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	843	GLN
1	A	1107	ASN
1	A	1112	GLN

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Mol	Chain	Res	Type
1	C	944	HIS
1	C	1107	ASN
1	D	955	GLN
1	D	988	ASN
1	D	1107	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	3O4	A	2229	-	32,32,32	1.52	4 (12%)	43,43,43	2.12	8 (18%)
2	3O4	B	2229	-	32,32,32	1.53	3 (9%)	43,43,43	2.17	8 (18%)
2	3O4	C	2229	-	32,32,32	1.53	3 (9%)	43,43,43	2.13	7 (16%)
2	3O4	D	2229	-	32,32,32	1.50	3 (9%)	43,43,43	2.19	8 (18%)

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	3O4	A	2229	-	-	0/16/24/24	0/4/4/4
2	3O4	B	2229	-	-	0/16/24/24	0/4/4/4
2	3O4	C	2229	-	-	0/16/24/24	0/4/4/4
2	3O4	D	2229	-	-	0/16/24/24	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2229	3O4	C16-C12	-5.77	1.40	1.48
2	A	2229	3O4	C16-C12	-5.76	1.40	1.48
2	C	2229	3O4	C16-C12	-5.72	1.40	1.48
2	D	2229	3O4	C16-C12	-5.64	1.40	1.48
2	C	2229	3O4	C25-N24	-3.80	1.34	1.41
2	B	2229	3O4	C25-N24	-3.78	1.34	1.41
2	D	2229	3O4	C25-N24	-3.77	1.34	1.41
2	A	2229	3O4	C25-N24	-3.73	1.34	1.41
2	C	2229	3O4	C1-N7	-2.83	1.34	1.40
2	D	2229	3O4	C1-N7	-2.78	1.34	1.40
2	B	2229	3O4	C1-N7	-2.76	1.34	1.40
2	A	2229	3O4	C1-N7	-2.74	1.34	1.40
2	A	2229	3O4	C9-N8	2.00	1.49	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2229	3O4	N15-C14-N13	-6.50	119.75	126.67
2	B	2229	3O4	N15-C14-N13	-6.48	119.76	126.67
2	A	2229	3O4	N15-C14-N13	-6.48	119.76	126.67
2	C	2229	3O4	N15-C14-N13	-6.31	119.94	126.67
2	C	2229	3O4	C11-C10-N15	-3.76	119.61	123.90
2	D	2229	3O4	C11-C10-N15	-3.55	119.84	123.90
2	A	2229	3O4	C11-C10-N15	-3.30	120.13	123.90
2	B	2229	3O4	C11-C10-N15	-3.25	120.19	123.90
2	B	2229	3O4	C11-C12-N13	-2.42	118.67	122.01
2	D	2229	3O4	C11-C12-N13	-2.36	118.76	122.01
2	A	2229	3O4	C11-C12-N13	-2.25	118.90	122.01
2	C	2229	3O4	C11-C12-N13	-2.19	119.00	122.01
2	B	2229	3O4	C25-N24-C22	-2.01	124.92	128.03
2	B	2229	3O4	O23-C22-N24	2.02	125.54	123.13
2	D	2229	3O4	O23-C22-N24	2.03	125.55	123.13
2	A	2229	3O4	O23-C22-N24	2.06	125.59	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2229	3O4	C16-C12-N13	2.60	119.59	116.13
2	D	2229	3O4	C16-C12-N13	3.23	120.43	116.13
2	C	2229	3O4	C16-C12-N13	3.50	120.78	116.13
2	C	2229	3O4	C9-N8-C28	3.55	119.05	111.59
2	A	2229	3O4	C9-N8-C28	3.88	119.73	111.59
2	B	2229	3O4	C9-N8-C28	4.01	120.00	111.59
2	D	2229	3O4	C9-N8-C28	4.46	120.96	111.59
2	C	2229	3O4	C12-N13-C14	6.01	120.98	116.49
2	B	2229	3O4	C10-N15-C14	6.38	121.03	115.49
2	D	2229	3O4	C12-N13-C14	6.58	121.40	116.49
2	A	2229	3O4	C10-N15-C14	6.68	121.29	115.49
2	A	2229	3O4	C12-N13-C14	6.75	121.53	116.49
2	D	2229	3O4	C10-N15-C14	7.00	121.57	115.49
2	C	2229	3O4	C10-N15-C14	7.16	121.72	115.49
2	B	2229	3O4	C12-N13-C14	7.54	122.11	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2229	3O4	3	0
2	B	2229	3O4	4	0
2	C	2229	3O4	3	0
2	D	2229	3O4	2	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	288/298 (96%)	1.50	70 (24%)  	15, 22, 37, 39	3 (1%)
1	B	288/298 (96%)	1.50	61 (21%)  	16, 23, 36, 37	3 (1%)
1	C	288/298 (96%)	1.44	56 (19%)  	16, 23, 35, 37	3 (1%)
1	D	288/298 (96%)	1.52	66 (22%)  	15, 22, 37, 39	3 (1%)
All	All	1152/1192 (96%)	1.49	253 (21%)  	15, 23, 36, 39	12 (1%)

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	871	LEU	10.4
1	C	1013	PRO	10.4
1	C	871	LEU	10.0
1	B	1013	PRO	9.2
1	A	871	LEU	8.9
1	D	871	LEU	7.5
1	A	1013	PRO	7.4
1	C	860	PHE	7.3
1	B	1014	GLY	7.2
1	B	1012	GLU	6.8
1	A	874	ASN	6.8
1	D	886	HIS	6.7
1	D	874	ASN	6.6
1	B	860	PHE	6.4
1	B	847	ARG	6.3
1	A	875	THR	6.3
1	D	1013	PRO	6.3
1	A	1014	GLY	6.3
1	B	875	THR	6.2
1	C	1012	GLU	6.2
1	B	874	ASN	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	886	HIS	6.0
1	D	1014	GLY	6.0
1	C	847	ARG	5.9
1	C	874	ASN	5.9
1	A	860	PHE	5.9
1	C	1053	LYS	5.8
1	D	875	THR	5.6
1	D	841	PRO	5.5
1	D	1011	LYS	5.2
1	D	847	ARG	5.2
1	C	875	THR	5.2
1	C	1014	GLY	5.1
1	B	1053	LYS	5.0
1	B	1011	LYS	5.0
1	A	842	THR	4.9
1	D	860	PHE	4.9
1	C	1092	ASP	4.8
1	D	949	ASP	4.8
1	C	1051	ILE	4.5
1	C	841	PRO	4.5
1	C	1070	GLN	4.5
1	A	847	ARG	4.5
1	B	971	ARG	4.5
1	A	1011	LYS	4.4
1	D	951	ILE	4.4
1	D	844	PHE	4.4
1	A	1008	TYR	4.3
1	B	945	LYS	4.3
1	D	1008	TYR	4.3
1	D	888	THR	4.2
1	A	1092	ASP	4.2
1	A	885	GLN	4.2
1	B	1051	ILE	4.1
1	D	1015	GLU	4.1
1	B	948	ILE	4.0
1	B	1092	ASP	4.0
1	C	971	ARG	3.9
1	A	1071	GLY	3.8
1	A	873	ASP	3.8
1	D	885	GLN	3.8
1	A	844	PHE	3.7
1	D	870	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	859	ASN	3.7
1	D	843	GLN	3.7
1	B	841	PRO	3.7
1	D	1092	ASP	3.7
1	D	920	ALA	3.6
1	A	859	ASN	3.6
1	B	951	ILE	3.6
1	D	1100	MET	3.6
1	D	1071	GLY	3.6
1	B	946	GLU	3.6
1	A	949	ASP	3.6
1	C	951	ILE	3.5
1	A	947	ARG	3.5
1	A	1004	ASP	3.5
1	A	841	PRO	3.5
1	A	861	GLY	3.4
1	B	1070	GLN	3.4
1	D	857	LYS	3.4
1	C	1100	MET	3.4
1	B	879	VAL	3.4
1	A	876	GLY	3.3
1	D	971	ARG	3.3
1	C	1128	ASP	3.3
1	B	1007	TYR	3.3
1	A	971	ARG	3.3
1	A	1100	MET	3.3
1	A	888	THR	3.3
1	C	862	SER	3.3
1	D	1012	GLU	3.2
1	C	859	ASN	3.2
1	B	1071	GLY	3.2
1	C	1000	VAL	3.2
1	B	1004	ASP	3.2
1	B	876	GLY	3.2
1	A	849	LEU	3.2
1	A	942	GLN	3.2
1	D	842	THR	3.2
1	A	1001	LEU	3.1
1	C	852	LEU	3.1
1	B	852	LEU	3.1
1	C	1071	GLY	3.1
1	C	1011	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	946	GLU	3.1
1	A	980	ARG	3.1
1	B	1000	VAL	3.0
1	A	1015	GLU	3.0
1	B	1100	MET	3.0
1	B	967	LEU	3.0
1	B	878	VAL	3.0
1	B	1117	ARG	3.0
1	B	1003	GLN	3.0
1	C	945	LYS	3.0
1	C	1010	VAL	2.9
1	A	1012	GLU	2.9
1	C	948	ILE	2.9
1	B	870	PRO	2.9
1	D	848	HIS	2.9
1	B	1010	VAL	2.9
1	D	918	TYR	2.9
1	B	842	THR	2.9
1	B	859	ASN	2.9
1	C	947	ARG	2.9
1	A	857	LYS	2.9
1	D	943	LYS	2.9
1	B	862	SER	2.8
1	D	861	GLY	2.8
1	D	881	VAL	2.8
1	D	1007	TYR	2.8
1	B	947	ARG	2.8
1	D	1070	GLN	2.8
1	D	967	LEU	2.7
1	A	881	VAL	2.7
1	C	878	VAL	2.7
1	C	1003	GLN	2.7
1	B	844	PHE	2.7
1	D	845	GLU	2.7
1	B	873	ASP	2.7
1	A	863	VAL	2.7
1	C	967	LEU	2.7
1	D	947	ARG	2.7
1	A	1007	TYR	2.6
1	C	1007	TYR	2.6
1	A	941	LEU	2.6
1	A	887	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	944	HIS	2.6
1	C	1004	ASP	2.6
1	C	1050	TYR	2.6
1	C	843	GLN	2.6
1	D	1000	VAL	2.6
1	A	951	ILE	2.6
1	B	866	CYS	2.6
1	C	1008	TYR	2.6
1	C	842	THR	2.6
1	A	1070	GLN	2.6
1	B	1050	TYR	2.6
1	D	1052	GLU	2.5
1	C	844	PHE	2.5
1	C	872	GLN	2.5
1	D	992	ILE	2.5
1	B	857	LYS	2.5
1	B	1005	LYS	2.5
1	C	942	GLN	2.5
1	B	1008	TYR	2.5
1	C	879	VAL	2.5
1	D	887	SER	2.5
1	D	925	LEU	2.5
1	D	863	VAL	2.4
1	A	920	ALA	2.4
1	A	870	PRO	2.4
1	A	852	LEU	2.4
1	A	1053	LYS	2.4
1	B	849	LEU	2.4
1	B	1047	LEU	2.4
1	C	1083	LYS	2.4
1	A	895	PHE	2.4
1	A	867	ARG	2.4
1	D	878	VAL	2.4
1	A	910	ILE	2.4
1	B	892	LEU	2.4
1	C	855	LEU	2.4
1	A	878	VAL	2.4
1	D	867	ARG	2.4
1	B	1017	PRO	2.3
1	D	1004	ASP	2.3
1	A	884	LEU	2.3
1	A	1000	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	876	GLY	2.3
1	B	887	SER	2.3
1	B	1033	VAL	2.3
1	D	910	ILE	2.3
1	B	865	MET	2.3
1	B	884	LEU	2.3
1	A	943	LYS	2.3
1	B	943	LYS	2.3
1	A	1128	ASP	2.2
1	A	1005	LYS	2.2
1	B	1101	ILE	2.2
1	A	1068	ASP	2.2
1	D	873	ASP	2.2
1	D	884	LEU	2.2
1	B	843	GLN	2.2
1	D	942	GLN	2.2
1	A	848	HIS	2.2
1	A	850	LYS	2.2
1	A	845	GLU	2.2
1	A	938	ARG	2.2
1	A	1121	LEU	2.2
1	C	929	MET	2.2
1	D	980	ARG	2.2
1	A	1067	ASN	2.2
1	D	941	LEU	2.2
1	D	862	SER	2.2
1	D	879	VAL	2.2
1	A	900	GLU	2.1
1	A	1106	TRP	2.1
1	A	1051	ILE	2.1
1	B	867	ARG	2.1
1	B	1083	LYS	2.1
1	D	876	GLY	2.1
1	D	921	GLY	2.1
1	D	1106	TRP	2.1
1	D	1019	PHE	2.1
1	A	918	TYR	2.1
1	A	967	LEU	2.1
1	D	852	LEU	2.1
1	C	848	HIS	2.1
1	C	857	LYS	2.1
1	C	887	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	945	LYS	2.1
1	C	1047	LEU	2.1
1	D	1001	LEU	2.1
1	B	890	GLU	2.1
1	A	851	PHE	2.1
1	B	1068	ASP	2.1
1	C	943	LYS	2.0
1	C	880	ALA	2.0
1	C	910	ILE	2.0
1	D	897	ARG	2.0
1	B	848	HIS	2.0
1	B	885	GLN	2.0
1	C	867	ARG	2.0
1	A	899	ILE	2.0
1	D	851	PHE	2.0
1	D	948	ILE	2.0
1	A	1052	GLU	2.0
1	D	931	TYR	2.0
1	A	879	VAL	2.0
1	C	870	PRO	2.0
1	C	1017	PRO	2.0
1	C	890	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
2	3O4	B	2229	29/29	0.80	0.20	0.05	32,32,32,32	0
2	3O4	D	2229	29/29	0.84	0.18	0.03	30,30,30,30	0
2	3O4	C	2229	29/29	0.82	0.20	0.03	32,32,32,32	0
2	3O4	A	2229	29/29	0.86	0.16	-0.18	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.