



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:42 AM GMT

PDB ID : 3FUP  
Title : Crystal structures of JAK1 and JAK2 inhibitor complexes  
Authors : Williams, N.K.; Bamert, R.S.; Patel, O.; Fantino, E.; Rossjohn, J.; Lucet, I.S.  
Deposited on : 2009-01-14  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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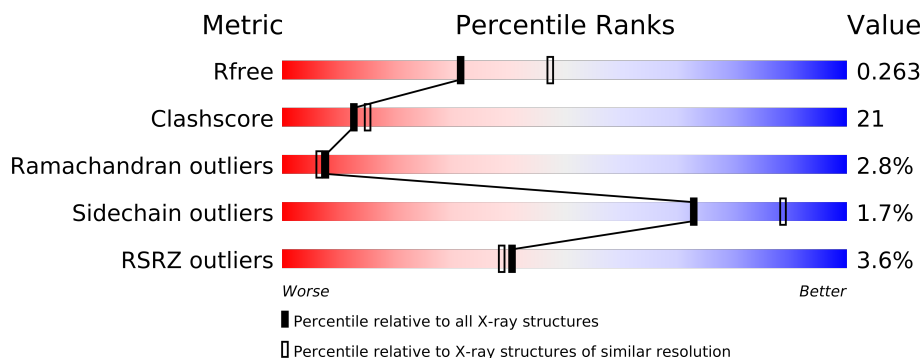
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	293	
1	B	293	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4938 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

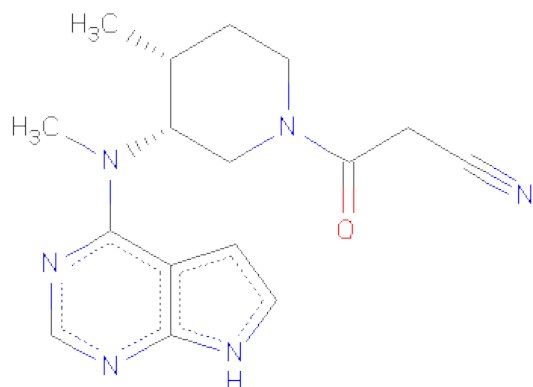
- Molecule 1 is a protein called Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	0
			2370	1504	407	443	2	14			
1	B	289	Total	C	N	O	P	S	0	0	0
			2387	1515	410	446	2	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1129	GLN	ASN	ENGINEERED	UNP O60674
B	1129	GLN	ASN	ENGINEERED	UNP O60674

- Molecule 2 is 3-[(3R,4R)-4-METHYL-3-[METHYL(7H-PYRROLO[2,3-D]PYRIMIDIN-4-YL)AMINO]PIPERIDIN-1-YL]-3-OXOPROPANENITRILE (three-letter code: MI1) (formula: C<sub>16</sub>H<sub>20</sub>N<sub>6</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	6	1		
2	B	1	Total	C	N	O	0	0
			23	16	6	1		

- Molecule 3 is water.

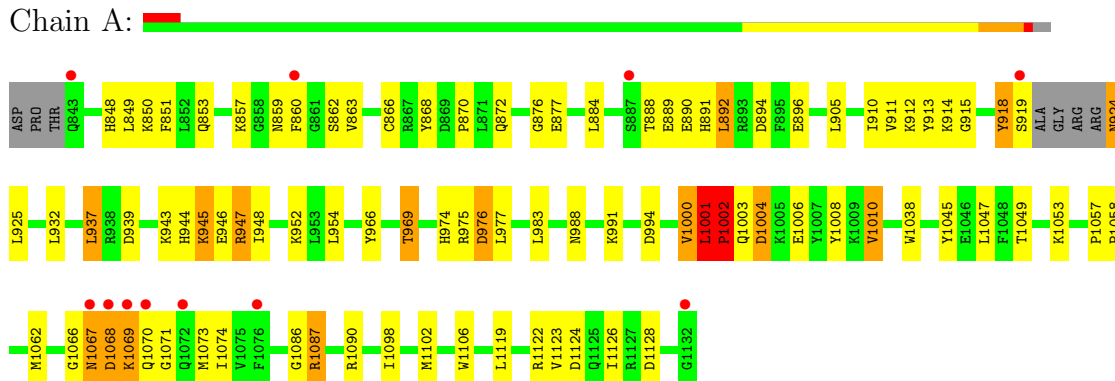
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	69	Total	O	0	0
			69	69		

### 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

Chain A:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.49Å 110.49Å 70.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.43 – 2.40 78.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (110.43-2.40) 94.4 (78.13-2.40)	Depositor EDS
$R_{merge}$	9.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.178 , 0.250 0.215 , 0.263	Depositor DCC
$R_{free}$ test set	1599 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.6	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 31434 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MI1, 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	0.80	0/2386	0.84	10/3208 (0.3%)
1	B	0.66	1/2404 (0.0%)	0.72	9/3234 (0.3%)
All	All	0.73	1/4790 (0.0%)	0.78	19/6442 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	16
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1045	TYR	CD2-CE2	5.48	1.47	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	924	ASN	O-C-N	-8.81	108.60	122.70
1	A	1087	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	924	ASN	CA-C-N	5.66	129.65	117.20
1	A	1128	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	949	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	1068	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	894	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	1004	ASP	CB-CG-OD2	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1068	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	939	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	976	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	1092	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	873	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	976	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	1124	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	1096	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	1004	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	869	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	1087	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1000	VAL	Peptide
1	A	1001	LEU	Peptide
1	A	1002	PRO	Peptide
1	A	892	LEU	Peptide
1	A	918	TYR	Peptide
1	A	945	LYS	Peptide
1	B	1010	VAL	Peptide
1	B	1071	GLY	Peptide
1	B	1072	GLN	Peptide
1	B	1095	PRO	Peptide
1	B	1096	ASP	Peptide
1	B	1097	GLU	Peptide
1	B	844	PHE	Peptide
1	B	899	ILE	Peptide
1	B	900	GLU	Peptide
1	B	941	LEU	Peptide
1	B	942	GLN	Peptide
1	B	943	LYS	Peptide
1	B	966	TYR	Peptide
1	B	967	LEU	Peptide
1	B	969	THR	Peptide
1	B	970	LYS	Peptide



## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2370	0	2334	69	2
1	B	2387	0	2345	123	1
2	A	23	0	18	7	0
2	B	23	0	20	5	0
3	A	66	0	0	3	0
3	B	69	0	0	8	0
All	All	4938	0	4717	199	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (199) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:944:HIS:HA	1:A:946:GLU:OE1	1.39	1.18
1:B:867:ARG:NH1	1:B:876:GLY:O	1.86	1.09
1:B:969:THR:O	1:B:969:THR:HG22	1.59	1.01
1:B:1071:GLY:O	1:B:1072:GLN:HG3	1.58	1.01
1:A:919:SER:C	1:A:924:ASN:HB2	1.84	0.97
1:A:1002:PRO:HD3	1:A:1008:PTR:HD2	1.48	0.94
1:B:1071:GLY:HA3	1:B:1073:MET:H	1.35	0.92
1:B:1068:ASP:O	1:B:1070:GLN:HG3	1.73	0.89
1:B:942:GLN:HG2	1:B:942:GLN:O	1.71	0.87
1:B:1093:GLY:O	1:B:1095:PRO:HD3	1.75	0.85
1:A:944:HIS:C	1:A:946:GLU:HB2	1.97	0.84
1:B:1122:ARG:HD2	3:B:113:HOH:O	1.77	0.84
1:A:1008:PTR:HE1	1:A:1010:VAL:HB	1.60	0.83
1:B:969:THR:O	1:B:970:LYS:HB2	1.78	0.82
1:B:897:ARG:O	1:B:901:ILE:HG12	1.80	0.81
1:B:1012:GLU:CG	3:B:82:HOH:O	2.29	0.80
1:A:892:LEU:C	1:A:892:LEU:HD23	2.01	0.80
2:A:1:MI1:H16	2:A:1:MI1:H1	1.63	0.80
1:B:1012:GLU:HG2	3:B:82:HOH:O	1.81	0.80
1:B:942:GLN:O	1:B:942:GLN:CG	2.31	0.78
1:B:985:GLU:OE1	1:B:989:ARG:HD2	1.83	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:969:THR:O	1:B:969:THR:CG2	2.30	0.78
1:B:1010:VAL:HG12	1:B:1011:LYS:H	1.48	0.77
1:B:873:ASP:OD1	1:B:875:THR:OG1	2.02	0.77
1:B:1102:MET:HE3	1:B:1106:TRP:CH2	2.20	0.75
1:A:1062:MET:HB3	1:A:1067:ASN:OD1	1.86	0.75
1:A:974:HIS:O	1:A:975:ARG:HB2	1.86	0.74
1:A:945:LYS:N	1:A:946:GLU:HB2	2.03	0.74
1:A:943:LYS:HD2	3:A:73:HOH:O	1.90	0.72
1:B:967:LEU:O	1:B:967:LEU:HD23	1.90	0.72
2:A:1:MI1:C16	2:A:1:MI1:H1	2.16	0.71
1:B:973:ILE:HG23	1:B:1032:SER:O	1.89	0.71
1:B:1097:GLU:H	1:B:1099:TYR:H	1.38	0.71
1:A:939:ASP:HB3	1:A:943:LYS:NZ	2.06	0.71
1:B:1071:GLY:C	1:B:1072:GLN:HG3	2.11	0.71
1:A:892:LEU:HD23	1:A:892:LEU:O	1.91	0.70
1:B:974:HIS:O	1:B:975:ARG:HB2	1.91	0.70
1:B:1057:PRO:HB2	1:B:1058:PRO:HD3	1.74	0.70
1:A:888:THR:HB	1:A:891:HIS:HB2	1.74	0.69
1:A:913:TYR:CZ	1:A:915:GLY:HA2	2.27	0.68
2:B:1:MI1:H16	2:B:1:MI1:H1	1.76	0.67
1:B:1010:VAL:CG1	1:B:1011:LYS:H	2.07	0.67
1:B:1008:PTR:O3P	1:B:1008:PTR:HE1	1.94	0.67
1:B:1095:PRO:HB2	1:B:1098:ILE:HG12	1.75	0.66
1:B:972:TYR:CE1	1:B:1000:VAL:HG22	2.31	0.66
1:A:966:TYR:O	1:A:969:THR:HB	1.96	0.65
1:A:1086:GLY:O	1:A:1087:ARG:HG3	1.97	0.65
1:B:1010:VAL:HG12	1:B:1011:LYS:N	2.08	0.65
1:A:1045:TYR:HB2	1:A:1102:MET:HE3	1.77	0.65
1:A:892:LEU:O	1:A:896:GLU:HG3	1.97	0.64
1:B:965:GLU:O	1:B:967:LEU:N	2.31	0.64
1:B:899:ILE:CD1	1:B:925:LEU:HD21	2.29	0.63
1:B:973:ILE:CG2	1:B:1032:SER:O	2.47	0.63
1:B:1012:GLU:HG3	3:B:82:HOH:O	1.95	0.63
1:B:898:GLU:O	1:B:900:GLU:N	2.30	0.62
1:A:918:TYR:HB3	1:A:919:SER:O	1.98	0.62
1:B:1068:ASP:O	1:B:1070:GLN:N	2.32	0.62
1:B:899:ILE:O	1:B:899:ILE:CG2	2.48	0.62
1:B:845:GLU:HG2	1:B:848:HIS:CE1	2.35	0.61
1:A:952:LYS:HE2	1:A:988:ASN:OD1	2.01	0.61
1:B:973:ILE:HD12	1:B:1032:SER:C	2.22	0.60
1:A:1057:PRO:HB2	1:A:1058:PRO:HD3	1.83	0.60
1:B:1102:MET:HE3	1:B:1106:TRP:HH2	1.63	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:852:LEU:HB2	1:B:865:MET:O	2.02	0.60
1:A:944:HIS:O	1:A:948:ILE:HD12	2.00	0.60
1:A:868:TYR:O	1:A:876:GLY:HA3	2.02	0.60
2:A:1:MI1:C16	2:A:1:MI1:C1	2.79	0.60
1:B:1086:GLY:O	1:B:1087:ARG:HD3	2.01	0.60
2:B:1:MI1:C16	2:B:1:MI1:H1	2.32	0.59
1:B:1096:ASP:CG	1:B:1096:ASP:O	2.40	0.59
1:B:943:LYS:H	1:B:945:LYS:H	1.48	0.59
1:B:974:HIS:HD2	1:B:976:ASP:H	1.50	0.59
1:B:913:TYR:CZ	1:B:915:GLY:HA2	2.38	0.59
1:B:983:LEU:HD21	2:B:1:MI1:H6	1.85	0.58
1:B:1125:GLN:O	1:B:1129:GLN:HG3	2.04	0.58
1:B:1010:VAL:CG1	1:B:1011:LYS:N	2.66	0.57
1:B:1060:GLU:CD	1:B:1063:ARG:HH21	2.07	0.57
1:A:918:TYR:HB3	1:A:919:SER:C	2.25	0.57
1:B:1109:ASN:HD22	1:B:1112:GLN:HE21	1.52	0.57
2:A:1:MI1:H16	2:A:1:MI1:C1	2.35	0.56
1:B:845:GLU:O	1:B:847:ARG:N	2.38	0.56
1:B:1098:ILE:N	1:B:1098:ILE:HD13	2.19	0.56
1:B:1068:ASP:O	1:B:1069:LYS:C	2.43	0.56
1:B:941:LEU:HD21	1:B:1047:LEU:HA	1.86	0.56
1:B:908:ASP:HB3	1:B:989:ARG:NH1	2.19	0.56
1:B:944:HIS:C	1:B:946:GLU:H	2.09	0.56
1:B:967:LEU:C	1:B:967:LEU:HD23	2.27	0.55
1:A:892:LEU:C	1:A:892:LEU:CD2	2.73	0.55
1:B:938:ARG:HD3	1:B:980:ARG:HB3	1.89	0.55
1:A:1004:ASP:N	1:A:1004:ASP:OD1	2.36	0.55
1:A:937:LEU:HD13	1:A:1047:LEU:HD21	1.89	0.54
2:A:1:MI1:H6	2:A:1:MI1:C16	2.38	0.54
1:B:950:HIS:CE1	1:B:1095:PRO:HD3	2.42	0.54
1:A:939:ASP:HB3	1:A:943:LYS:HZ1	1.72	0.54
1:A:1069:LYS:O	1:A:1070:GLN:NE2	2.40	0.53
1:A:954:LEU:HD21	1:A:1098:ILE:HD12	1.90	0.53
1:B:1068:ASP:OD1	1:B:1069:LYS:N	2.41	0.53
1:B:1090:ARG:HG2	1:B:1094:CYS:HB3	1.91	0.53
1:B:967:LEU:CD2	1:B:972:TYR:HB2	2.38	0.53
1:A:932:LEU:HD11	1:A:991:LYS:HD2	1.90	0.53
1:B:1068:ASP:O	1:B:1070:GLN:CG	2.53	0.52
1:B:845:GLU:O	1:B:846:GLU:C	2.47	0.52
1:B:966:TYR:O	1:B:966:TYR:CG	2.63	0.51
1:B:950:HIS:C	1:B:952:LYS:H	2.12	0.51
1:B:974:HIS:HE1	1:B:994:ASP:O	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:905:LEU:HD13	1:A:910:ILE:HD13	1.93	0.51
1:B:965:GLU:C	1:B:967:LEU:H	2.13	0.51
1:A:863:VAL:CG2	2:A:1:MI1:O21	2.59	0.51
1:B:844:PHE:CD2	1:B:928:ILE:HG13	2.46	0.50
1:B:852:LEU:HD12	1:B:865:MET:HG2	1.94	0.50
1:B:974:HIS:O	1:B:975:ARG:CB	2.60	0.50
1:A:848:HIS:CG	1:A:870:PRO:HA	2.47	0.50
1:B:941:LEU:HD11	1:B:953:LEU:HD21	1.93	0.49
1:B:972:TYR:HE1	1:B:1000:VAL:HG22	1.77	0.49
1:B:1048:PHE:CE2	1:B:1098:ILE:HG21	2.47	0.49
1:A:945:LYS:N	1:A:946:GLU:CB	2.74	0.49
1:B:944:HIS:C	1:B:946:GLU:N	2.66	0.49
1:B:898:GLU:C	1:B:900:GLU:N	2.66	0.49
1:B:899:ILE:HD12	1:B:925:LEU:HD21	1.94	0.48
1:A:1053:LYS:HB2	3:A:108:HOH:O	2.12	0.48
1:B:854:GLN:HG3	1:B:855:LEU:N	2.28	0.48
1:B:961:CYS:SG	1:B:1040:PHE:CZ	3.07	0.48
1:A:1066:GLY:C	1:A:1068:ASP:H	2.17	0.48
1:A:877:GLU:OE2	1:A:914:LYS:HE3	2.13	0.48
1:A:860:PHE:O	1:A:884:LEU:HD23	2.14	0.48
1:A:850:LYS:O	1:A:866:CYS:HA	2.14	0.47
1:B:1002:PRO:HG2	1:B:1005:LYS:HB2	1.96	0.47
1:A:974:HIS:HD2	1:A:976:ASP:H	1.62	0.47
1:A:1102:MET:HE3	1:A:1106:TRP:HH2	1.79	0.47
1:A:1001:LEU:C	1:A:1002:PRO:O	2.52	0.47
1:B:974:HIS:CE1	1:B:994:ASP:O	2.67	0.47
1:B:1099:TYR:CD1	1:B:1102:MET:HE2	2.50	0.47
1:B:975:ARG:HD3	1:B:997:LEU:O	2.14	0.47
1:A:888:THR:HG22	1:A:890:GLU:H	1.80	0.47
1:A:1008:PTR:O2P	1:A:1008:PTR:HE2	2.13	0.46
1:A:944:HIS:HA	1:A:946:GLU:CD	2.28	0.46
1:A:974:HIS:HE1	1:A:994:ASP:O	1.98	0.46
1:A:1122:ARG:O	1:A:1126:ILE:HG13	2.15	0.46
1:A:1071:GLY:HA2	1:A:1074:ILE:HD12	1.97	0.46
1:B:907:HIS:HE1	1:B:909:ASN:HD22	1.62	0.46
1:A:1003:GLN:HG2	1:A:1003:GLN:O	2.16	0.46
1:B:1008:PTR:O3P	1:B:1008:PTR:CE1	2.64	0.45
1:A:1102:MET:HE3	1:A:1106:TRP:CH2	2.51	0.45
1:B:965:GLU:C	1:B:967:LEU:N	2.67	0.45
1:B:1091:PRO:HB2	1:B:1094:CYS:HB2	1.97	0.45
1:A:1090:ARG:HH22	1:B:1122:ARG:NH1	2.14	0.45
1:B:952:LYS:NZ	1:B:988:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1:MI1:C16	2:B:1:MI1:C1	2.94	0.45
1:A:1008:PTR:CD1	1:A:1008:PTR:C	2.94	0.45
1:B:967:LEU:HD23	1:B:972:TYR:HB2	1.99	0.45
1:B:899:ILE:O	1:B:899:ILE:HG22	2.16	0.45
1:A:888:THR:HG22	1:A:889:GLU:N	2.31	0.45
1:B:1093:GLY:O	1:B:1095:PRO:CD	2.55	0.45
1:A:857:LYS:HG2	1:A:862:SER:HB2	1.99	0.45
1:B:964:MET:O	1:B:967:LEU:HB3	2.17	0.44
1:A:1038:TRP:CE3	1:A:1106:TRP:HA	2.52	0.44
1:A:919:SER:HB3	1:A:924:ASN:HA	1.99	0.44
1:B:950:HIS:C	1:B:952:LYS:N	2.71	0.44
1:A:983:LEU:HD13	2:A:1:MI1:H7A	1.99	0.44
1:A:974:HIS:CE1	1:A:994:ASP:O	2.71	0.43
1:A:1045:TYR:O	1:A:1049:THR:HG23	2.18	0.43
1:B:1065:ILE:HG22	1:B:1065:ILE:O	2.19	0.43
1:B:848:HIS:HD2	1:B:872:GLN:NE2	2.17	0.43
1:B:941:LEU:CD2	1:B:1047:LEU:HA	2.49	0.43
1:B:955:GLN:NE2	3:B:107:HOH:O	2.51	0.43
1:A:1119:LEU:O	1:A:1123:VAL:HG23	2.19	0.43
1:A:849:LEU:HA	1:A:849:LEU:HD12	1.86	0.43
1:B:1071:GLY:CA	1:B:1073:MET:H	2.19	0.42
1:A:851:PHE:CZ	1:A:853:GLN:HA	2.54	0.42
1:B:1099:TYR:CD1	1:B:1102:MET:CE	3.02	0.42
1:B:1025:SER:HA	1:B:1030:LYS:H	1.84	0.42
1:B:918:TYR:CE1	1:B:925:LEU:HD13	2.54	0.42
1:B:1090:ARG:CG	1:B:1094:CYS:HB3	2.50	0.42
1:B:972:TYR:CD1	1:B:1000:VAL:HG22	2.54	0.42
1:B:950:HIS:O	1:B:952:LYS:N	2.53	0.42
1:B:846:GLU:OE1	1:B:926:LYS:NZ	2.47	0.42
1:A:911:VAL:HG22	1:A:912:LYS:H	1.85	0.42
1:A:913:TYR:CZ	1:A:915:GLY:CA	3.02	0.42
1:B:1094:CYS:HA	1:B:1095:PRO:HD2	1.88	0.41
1:B:899:ILE:O	1:B:899:ILE:HG23	2.20	0.41
1:B:898:GLU:C	1:B:900:GLU:H	2.21	0.41
1:B:846:GLU:CD	1:B:926:LYS:HZ3	2.23	0.41
1:B:935:GLY:HA2	3:B:16:HOH:O	2.21	0.41
1:B:848:HIS:CD2	1:B:870:PRO:HA	2.56	0.41
1:B:1032:SER:HB2	3:B:13:HOH:O	2.20	0.41
1:A:913:TYR:OH	1:A:915:GLY:HA2	2.20	0.41
1:B:983:LEU:HD21	2:B:1:MI1:C6	2.51	0.41
1:B:917:CYS:SG	1:B:926:LYS:HE3	2.61	0.41
1:B:966:TYR:O	1:B:966:TYR:CD1	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:951:ILE:HG22	3:B:2:HOH:O	2.21	0.41
1:B:1009:LYS:HA	1:B:1029:SER:O	2.21	0.41
1:B:970:LYS:O	1:B:972:TYR:N	2.54	0.41
1:B:1057:PRO:CB	1:B:1058:PRO:HD3	2.47	0.41
1:A:1006:GLU:OE1	3:A:59:HOH:O	2.22	0.41
1:A:1001:LEU:HA	1:A:1002:PRO:HD2	1.14	0.40
1:A:977:LEU:HA	1:A:977:LEU:HD23	1.90	0.40
1:B:1069:LYS:O	1:B:1074:ILE:CG1	2.69	0.40
1:B:931:TYR:CZ	1:B:933:PRO:HA	2.57	0.40
1:B:1099:TYR:HD1	1:B:1102:MET:CE	2.34	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:947:ARG:NH2	1:B:989:ARG:NH2[4.454]	1.66	0.54
1:A:872:GLN:O	1:A:1073:MET:SD[2.454]	2.15	0.05

## 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	280/293 (96%)	263 (94%)	12 (4%)	5 (2%)	13	15
1	B	283/293 (97%)	251 (89%)	21 (7%)	11 (4%)	5	3
All	All	563/586 (96%)	514 (91%)	33 (6%)	16 (3%)	8	6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1002	PRO
1	A	1069	LYS
1	B	901	ILE
1	B	943	LYS
1	B	970	LYS

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Mol	Chain	Res	Type
1	B	1013	PRO
1	B	1069	LYS
1	B	945	LYS
1	B	1097	GLU
1	B	899	ILE
1	B	966	TYR
1	B	1072	GLN
1	B	1095	PRO
1	A	1067	ASN
1	A	859	ASN
1	A	1001	LEU

### 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	259/265 (98%)	253 (98%)	6 (2%)	63	82
1	B	260/265 (98%)	257 (99%)	3 (1%)	82	93
All	All	519/530 (98%)	510 (98%)	9 (2%)	73	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	925	LEU
1	A	937	LEU
1	A	947	ARG
1	A	969	THR
1	A	1000	VAL
1	A	1010	VAL
1	B	875	THR
1	B	944	HIS
1	B	1054	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	885	GLN
1	A	909	ASN
1	A	942	GLN
1	A	955	GLN
1	A	974	HIS
1	A	1070	GLN
1	B	848	HIS
1	B	854	GLN
1	B	909	ASN
1	B	944	HIS
1	B	955	GLN
1	B	974	HIS
1	B	1112	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PTR	A	1007	1	16,16,17	4.76	3 (18%)	20,22,24	0.77	1 (5%)
1	PTR	A	1008	1	16,16,17	4.79	3 (18%)	20,22,24	0.75	1 (5%)
1	PTR	B	1007	1	16,16,17	4.78	3 (18%)	20,22,24	0.65	1 (5%)
1	PTR	B	1008	1	16,16,17	4.78	3 (18%)	20,22,24	0.75	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	A	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1008	1	-	0/9/11/13	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1008	PTR	O-C	17.70	1.23	1.11
1	B	1008	PTR	O-C	17.68	1.23	1.11
1	B	1007	PTR	O-C	17.68	1.23	1.11
1	A	1007	PTR	O-C	17.59	1.23	1.11
1	A	1008	PTR	OH-CZ	-6.76	1.23	1.40
1	B	1007	PTR	OH-CZ	-6.74	1.23	1.40
1	B	1008	PTR	OH-CZ	-6.71	1.23	1.40
1	A	1007	PTR	OH-CZ	-6.70	1.23	1.40
1	A	1008	PTR	CA-C	2.50	1.52	1.48
1	A	1007	PTR	CA-C	2.50	1.52	1.48
1	B	1008	PTR	CA-C	2.49	1.52	1.48
1	B	1007	PTR	CA-C	2.48	1.52	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1007	PTR	C-CA-N	-2.71	111.12	113.83
1	A	1008	PTR	C-CA-N	-2.62	111.21	113.83
1	B	1008	PTR	C-CA-N	-2.61	111.22	113.83
1	B	1007	PTR	C-CA-N	-2.03	111.81	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	MI1	A	1	-	25,25,25	2.61	3 (12%)	33,35,35	2.88	14 (42%)
2	MI1	B	1	-	25,25,25	2.19	2 (8%)	33,35,35	2.78	17 (51%)

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	MI1	A	1	-	-	0/15/28/28	0/1/3/3
2	MI1	B	1	-	-	0/15/28/28	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	MI1	C22-C23	-10.12	1.27	1.45
2	B	1	MI1	C22-C23	-8.52	1.30	1.45
2	A	1	MI1	C22-C20	-6.65	1.46	1.52
2	B	1	MI1	C22-C20	-5.18	1.48	1.52
2	A	1	MI1	C20-N3	-2.11	1.30	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	MI1	N17-C18-N19	-9.49	120.77	128.71
2	B	1	MI1	N17-C18-N19	-6.89	122.95	128.71
2	B	1	MI1	C22-C23-N24	-6.58	153.04	177.68
2	A	1	MI1	C18-N19-C10	5.50	123.46	111.53
2	A	1	MI1	N12-C14-N17	5.08	134.36	125.34
2	B	1	MI1	N12-C14-N17	5.07	134.34	125.34
2	B	1	MI1	C18-N19-C10	4.72	121.77	111.53
2	B	1	MI1	C4-N3-C2	4.24	122.52	113.22
2	A	1	MI1	C23-C22-C20	4.14	119.40	111.49
2	A	1	MI1	C6-C1-N8	-3.47	108.19	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	MI1	C4-N3-C2	3.44	120.77	113.22
2	A	1	MI1	C18-N17-C14	3.31	121.30	114.82
2	B	1	MI1	C7-C6-C1	3.25	118.93	113.48
2	B	1	MI1	C15-C14-N17	-3.13	119.41	125.19
2	A	1	MI1	C10-N8-C1	-3.11	117.92	121.03
2	B	1	MI1	C23-C22-C20	3.04	117.30	111.49
2	B	1	MI1	C9-N8-C1	2.93	122.22	118.03
2	A	1	MI1	C9-N8-C1	2.85	122.11	118.03
2	A	1	MI1	C15-C14-N17	-2.79	120.03	125.19
2	B	1	MI1	C18-N17-C14	2.78	120.26	114.82
2	A	1	MI1	C22-C23-N24	-2.76	167.33	177.68
2	A	1	MI1	C16-C11-N12	2.70	112.73	108.17
2	B	1	MI1	C2-N3-C20	-2.56	114.19	122.92
2	B	1	MI1	C15-C10-N19	-2.47	118.08	123.51
2	A	1	MI1	N19-C10-N8	2.34	119.52	116.95
2	B	1	MI1	C7-C6-C5	-2.34	106.81	110.85
2	B	1	MI1	C6-C1-N8	-2.30	109.79	112.93
2	B	1	MI1	C16-C11-N12	2.25	111.96	108.17
2	A	1	MI1	C15-C10-N19	-2.21	118.67	123.51
2	B	1	MI1	C22-C20-N3	2.05	121.11	117.57
2	B	1	MI1	O21-C20-N3	-2.04	117.27	121.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	286/293 (97%)	0.27	11 (3%) 38 36	24, 39, 73, 106	0
1	B	289/293 (98%)	0.29	10 (3%) 42 40	30, 41, 71, 116	0
All	All	575/586 (98%)	0.28	21 (3%) 41 38	24, 40, 73, 116	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1068	ASP	8.3
1	B	1013	PRO	6.1
1	A	1067	ASN	5.6
1	A	1069	LYS	5.0
1	A	860	PHE	4.8
1	A	1070	GLN	4.5
1	A	919	SER	4.4
1	B	1069	LYS	4.3
1	B	1053	LYS	4.2
1	A	1072	GLN	4.0
1	B	1071	GLY	3.9
1	B	877	GLU	3.5
1	B	847	ARG	3.3
1	A	843	GLN	3.0
1	B	941	LEU	2.9
1	A	887	SER	2.8
1	A	1132	GLY	2.7
1	B	1070	GLN	2.5
1	B	1067	ASN	2.3
1	A	1076	PHE	2.2
1	B	1068	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	B	1008	16/17	0.18	0.27	42,59,78,81	0
1	PTR	A	1008	16/17	0.14	-0.71	28,56,67,67	0
1	PTR	B	1007	16/17	0.13	-1.63	43,58,77,82	0
1	PTR	A	1007	16/17	0.10	-2.25	32,43,64,67	0

## 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MI1	B	1	23/23	0.18	0.49	28,35,48,55	0
2	MI1	A	1	23/23	0.16	-0.09	26,40,44,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.