



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:45 PM GMT

PDB ID : 1Q7F  
Title : Brain Tumor NHL domain  
Authors : Edwards, T.A.; Wilkinson, B.D.; Wharton, R.P.; Aggarwal, A.K.  
Deposited on : 2003-08-18  
Resolution : 1.95 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>

---

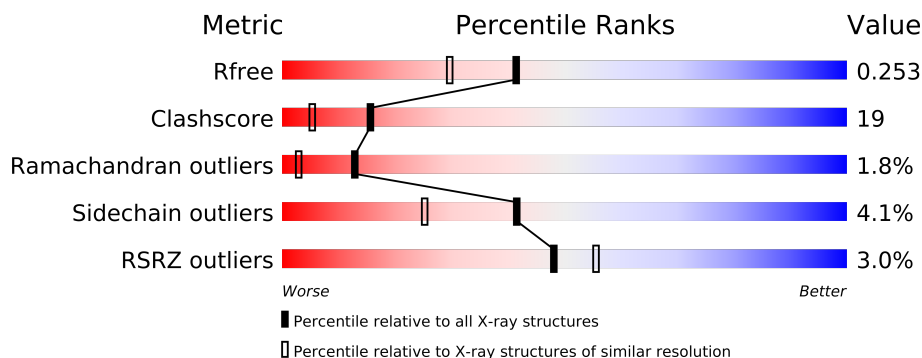
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.95 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	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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	286	
1	B	286	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5138 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 brain tumor CG10719-PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2227	1409	400	407	11			
1	B	282	Total	C	N	O	S	0	0	0
			2251	1423	405	412	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	GLY	-	CLONING ARTIFACT	UNP Q8MQJ9
A	753	THR	-	CLONING ARTIFACT	UNP Q8MQJ9
A	754	HIS	-	CLONING ARTIFACT	UNP Q8MQJ9
A	755	MET	-	CLONING ARTIFACT	UNP Q8MQJ9
A	763	ARG	LYS	CONFLICT	UNP Q8MQJ9
B	752	GLY	-	CLONING ARTIFACT	UNP Q8MQJ9
B	753	THR	-	CLONING ARTIFACT	UNP Q8MQJ9
B	754	HIS	-	CLONING ARTIFACT	UNP Q8MQJ9
B	755	MET	-	CLONING ARTIFACT	UNP Q8MQJ9
B	763	ARG	LYS	CONFLICT	UNP Q8MQJ9

- Molecule 2 is water.

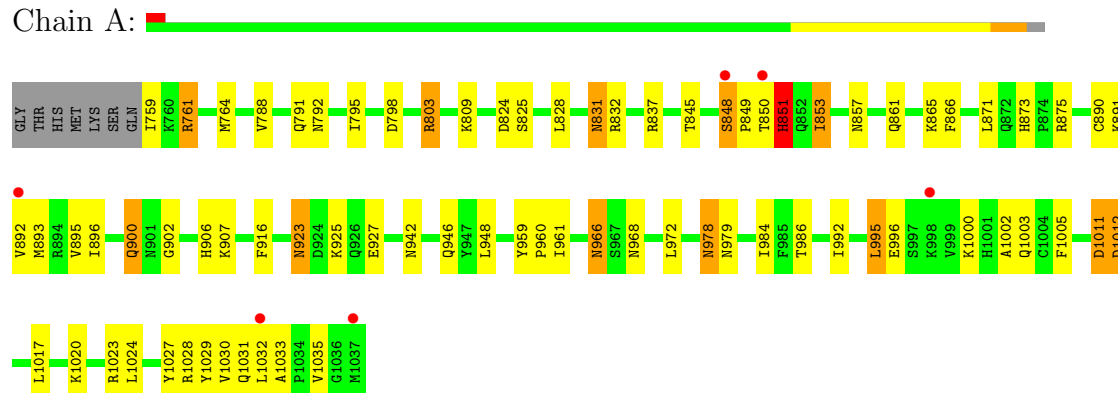
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	334	Total	O	0	0
			334	334		
2	B	326	Total	O	0	0
			326	326		

### 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.

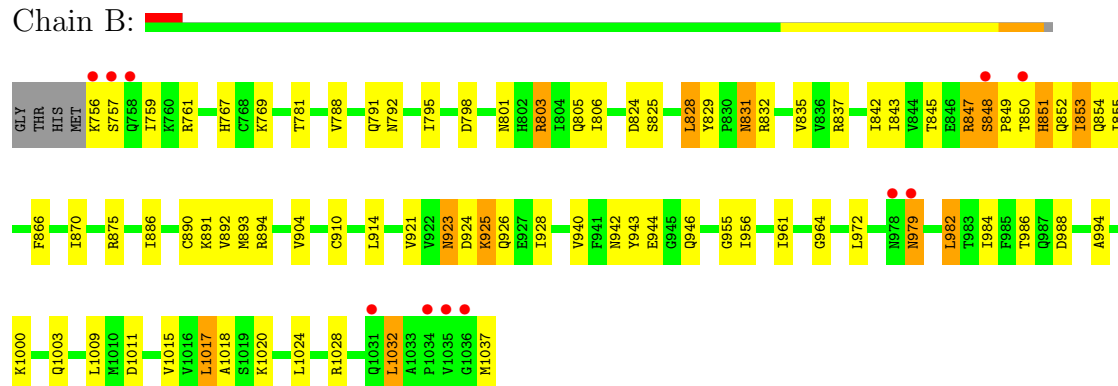
#### • Molecule 1: brain tumor CG10719-PA

Chain A:



#### • Molecule 1: brain tumor CG10719-PA

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.77Å 94.58Å 130.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 39.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.6 (15.00-1.95) 80.3 (39.29-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.50 (at 1.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.200 , 0.252 0.200 , 0.253	Depositor DCC
$R_{free}$ test set	1425 reflections (4.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 37486 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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

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	0.36	0/2270	0.65	1/3060 (0.0%)
1	B	0.35	0/2294	0.64	0/3091
All	All	0.35	0/4564	0.65	1/6151 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	978	ASN	N-CA-C	-5.56	95.98	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2227	0	2202	85	0
1	B	2251	0	2228	84	0
2	A	334	0	0	13	0
2	B	326	0	0	9	0
All	All	5138	0	4430	166	0

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 19.

All (166) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1032:LEU:H	1:B:1032:LEU:HD12	1.21	1.01
1:A:857:ASN:HD21	1:A:861:GLN:HE21	1.19	0.87
1:B:924:ASP:O	1:B:925:LYS:HG3	1.76	0.86
1:A:1032:LEU:O	1:A:1032:LEU:HD13	1.85	0.75
1:B:831:ASN:HD22	1:B:831:ASN:H	1.34	0.75
1:B:1003:GLN:HB3	1:B:1020:LYS:HE3	1.70	0.74
1:A:873:HIS:NE2	1:A:891:LYS:HD3	2.02	0.74
1:A:942:ASN:HD21	1:A:946:GLN:HB2	1.54	0.71
1:A:986:THR:CG2	1:A:992:ILE:HD11	2.20	0.71
1:B:757:SER:HB2	2:B:144:HOH:O	1.91	0.69
1:A:1028:ARG:HH22	1:A:1032:LEU:HD23	1.59	0.68
1:A:942:ASN:ND2	1:A:946:GLN:HB2	2.09	0.68
1:A:857:ASN:HD21	1:A:861:GLN:NE2	1.91	0.67
1:B:1017:LEU:HD23	1:B:1018:ALA:N	2.10	0.66
1:A:1028:ARG:NH2	1:A:1032:LEU:HD23	2.11	0.65
1:A:906:HIS:CD2	1:A:907:LYS:H	2.14	0.65
1:B:855:ILE:N	1:B:855:ILE:HD12	2.12	0.65
1:A:1028:ARG:HH11	1:A:1028:ARG:HG3	1.61	0.64
1:A:978:ASN:O	1:A:979:ASN:HB2	1.97	0.64
1:B:1032:LEU:H	1:B:1032:LEU:CD1	2.00	0.63
1:A:986:THR:HG23	1:A:992:ILE:HD11	1.81	0.62
1:A:831:ASN:O	1:A:831:ASN:ND2	2.32	0.62
1:A:1029:TYR:CD1	1:A:1030:VAL:HG13	2.33	0.62
1:A:900:GLN:HB2	2:A:88:HOH:O	2.00	0.62
1:A:1000:LYS:NZ	1:B:994:ALA:HB3	2.16	0.61
1:B:853:ILE:HG23	1:B:866:PHE:O	2.01	0.60
1:B:759:ILE:CD1	1:B:956:ILE:HG23	2.30	0.60
1:B:875:ARG:HG3	1:B:890:CYS:SG	2.41	0.60
1:A:857:ASN:ND2	1:A:861:GLN:HE21	1.96	0.60
1:B:853:ILE:HD12	1:B:854:GLN:N	2.16	0.60
1:A:761:ARG:CZ	2:A:9:HOH:O	2.48	0.60
1:A:986:THR:HG22	1:A:992:ILE:HD11	1.84	0.60
1:B:910:CYS:SG	1:B:914:LEU:HD12	2.41	0.60
1:B:972:LEU:HD22	1:B:984:ILE:HG23	1.84	0.60
1:A:1028:ARG:NH2	1:A:1032:LEU:HB2	2.16	0.59
1:B:781:THR:HG23	1:B:801:ASN:ND2	2.17	0.59
1:B:1017:LEU:C	1:B:1017:LEU:HD23	2.23	0.58
1:A:828:LEU:HD23	1:A:850:THR:OG1	2.04	0.58
1:A:761:ARG:HG3	1:A:996:GLU:OE1	2.05	0.57
1:A:831:ASN:O	1:A:832:ARG:HB2	2.05	0.57
1:B:1032:LEU:N	1:B:1032:LEU:HD12	2.05	0.57
1:A:795:ILE:N	1:A:795:ILE:HD12	2.20	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:892:VAL:O	1:A:892:VAL:HG12	2.04	0.57
1:A:923:ASN:C	1:A:923:ASN:HD22	2.07	0.57
1:A:848:SER:HB3	1:A:849:PRO:HD3	1.85	0.56
1:B:806:ILE:N	1:B:806:ILE:HD12	2.21	0.56
1:B:870:ILE:HD13	1:B:904:VAL:HG21	1.88	0.56
1:B:942:ASN:ND2	1:B:946:GLN:HG2	2.21	0.56
1:B:848:SER:HB3	1:B:849:PRO:HD3	1.88	0.56
1:B:824:ASP:O	1:B:825:SER:HB2	2.06	0.56
1:A:1035:VAL:HG23	2:A:653:HOH:O	2.04	0.56
1:A:824:ASP:O	1:A:825:SER:HB2	2.07	0.55
1:B:923:ASN:C	1:B:923:ASN:HD22	2.09	0.55
1:B:854:GLN:C	1:B:855:ILE:HD12	2.26	0.55
1:B:837:ARG:HH11	1:B:837:ARG:HG3	1.72	0.55
1:B:831:ASN:N	1:B:831:ASN:HD22	2.04	0.55
1:B:849:PRO:HG2	2:B:478:HOH:O	2.05	0.55
1:A:892:VAL:HB	2:A:145:HOH:O	2.06	0.55
1:B:926:GLN:HG2	1:B:943:TYR:CE2	2.42	0.55
1:A:837:ARG:NH1	2:A:54:HOH:O	2.39	0.54
1:B:886:ILE:N	1:B:886:ILE:HD12	2.22	0.54
1:B:849:PRO:HG3	2:B:550:HOH:O	2.08	0.54
1:A:961:ILE:HD12	1:A:961:ILE:C	2.27	0.54
1:A:1028:ARG:NH1	1:A:1028:ARG:HG3	2.23	0.53
1:A:890:CYS:C	1:A:892:VAL:H	2.13	0.52
1:A:875:ARG:HD2	2:A:437:HOH:O	2.09	0.52
1:A:972:LEU:HD13	1:A:984:ILE:HG23	1.92	0.52
1:B:798:ASP:OD2	1:B:803:ARG:HD2	2.10	0.52
1:B:795:ILE:HD12	1:B:835:VAL:CG2	2.40	0.52
1:A:923:ASN:ND2	1:A:925:LYS:H	2.08	0.52
1:B:837:ARG:NH1	1:B:837:ARG:HG3	2.25	0.52
1:B:850:THR:O	1:B:852:GLN:N	2.43	0.52
1:B:791:GLN:O	1:B:792:ASN:HB2	2.10	0.52
1:B:788:VAL:CG1	1:B:792:ASN:HA	2.40	0.51
1:B:1009:LEU:N	1:B:1009:LEU:HD12	2.26	0.51
1:B:1003:GLN:CB	1:B:1020:LYS:HE3	2.39	0.51
1:A:995:LEU:N	1:A:995:LEU:HD22	2.26	0.50
1:B:921:VAL:HG11	1:B:964:GLY:HA2	1.93	0.50
1:A:764:MET:HE2	1:A:1027:TYR:HB3	1.93	0.50
1:B:890:CYS:HB2	2:B:564:HOH:O	2.12	0.50
1:B:942:ASN:HD21	1:B:946:GLN:HG2	1.77	0.50
1:B:1017:LEU:C	1:B:1017:LEU:CD2	2.80	0.50
1:B:1018:ALA:HA	1:B:1024:LEU:HD13	1.94	0.50
1:A:849:PRO:HA	2:A:106:HOH:O	2.12	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:756:LYS:N	2:B:224:HOH:O	2.45	0.50
1:B:972:LEU:HD23	1:B:972:LEU:N	2.27	0.49
1:A:871:LEU:HD23	1:A:896:ILE:HD12	1.93	0.49
1:A:831:ASN:HD22	1:A:831:ASN:H	1.57	0.49
1:B:756:LYS:O	1:B:955:GLY:HA2	2.12	0.49
1:A:764:MET:CE	1:A:1027:TYR:HB3	2.43	0.49
1:A:832:ARG:HD2	2:A:58:HOH:O	2.12	0.49
1:B:972:LEU:HG	1:B:1009:LEU:HD21	1.95	0.48
1:B:843:ILE:HG23	1:B:853:ILE:CD1	2.44	0.48
1:A:831:ASN:O	1:A:845:THR:OG1	2.32	0.48
1:B:972:LEU:CD2	1:B:984:ILE:HG23	2.44	0.48
1:A:850:THR:O	1:A:850:THR:HG22	2.14	0.48
1:A:792:ASN:HD21	1:A:1011:ASP:H	1.62	0.48
1:A:923:ASN:HD21	1:A:927:GLU:H	1.61	0.48
1:A:972:LEU:CD1	1:A:984:ILE:HG12	2.44	0.48
1:A:959:TYR:N	1:A:960:PRO:CD	2.77	0.48
1:A:848:SER:O	1:A:851:HIS:CD2	2.66	0.47
1:A:1023:ARG:NH1	1:B:1037:MET:HE3	2.29	0.47
1:B:832:ARG:HB2	1:B:845:THR:OG1	2.14	0.47
1:B:805:GLN:C	1:B:806:ILE:HD12	2.35	0.47
1:B:769:LYS:HG2	2:B:52:HOH:O	2.14	0.47
1:A:1023:ARG:HH11	1:A:1023:ARG:HG3	1.79	0.47
1:A:873:HIS:CD2	1:A:891:LYS:HD3	2.49	0.47
1:B:1028:ARG:HD2	2:B:227:HOH:O	2.15	0.47
1:A:942:ASN:HD22	1:A:948:LEU:HD21	1.80	0.46
1:B:979:ASN:HA	2:B:13:HOH:O	2.14	0.46
1:A:853:ILE:HD11	1:A:866:PHE:CZ	2.50	0.46
1:B:1020:LYS:O	1:B:1020:LYS:HG2	2.15	0.46
1:A:798:ASP:OD2	1:A:803:ARG:HD2	2.16	0.46
1:A:792:ASN:HB2	1:A:809:LYS:HE2	1.98	0.46
1:A:1002:ALA:O	1:A:1003:GLN:C	2.53	0.46
1:A:865:LYS:NZ	2:A:103:HOH:O	2.49	0.46
1:A:923:ASN:ND2	1:A:923:ASN:C	2.69	0.46
1:B:781:THR:HG23	1:B:801:ASN:HD21	1.80	0.46
1:B:847:ARG:HG2	1:B:848:SER:N	2.29	0.46
1:B:890:CYS:O	1:B:892:VAL:HG22	2.16	0.45
1:B:942:ASN:ND2	1:B:944:GLU:OE1	2.50	0.45
1:A:875:ARG:HG3	1:A:890:CYS:SG	2.57	0.45
1:A:972:LEU:HD13	1:A:984:ILE:HG12	1.98	0.45
1:B:759:ILE:HD11	1:B:956:ILE:HG23	1.98	0.45
1:B:792:ASN:HD21	1:B:1011:ASP:H	1.64	0.45
1:A:1011:ASP:O	1:A:1012:ASP:HB3	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:761:ARG:HD3	1:A:996:GLU:HB3	1.98	0.44
1:A:849:PRO:HD2	2:A:155:HOH:O	2.17	0.44
1:B:832:ARG:CZ	2:B:420:HOH:O	2.65	0.44
1:B:761:ARG:HG2	1:B:994:ALA:HB1	2.00	0.44
1:B:892:VAL:HG23	1:B:894:ARG:HG2	2.00	0.44
1:A:791:GLN:O	1:A:792:ASN:HB2	2.17	0.44
1:B:961:ILE:C	1:B:961:ILE:HD12	2.37	0.44
1:B:891:LYS:HG2	1:B:891:LYS:O	2.18	0.43
1:B:828:LEU:HD12	1:B:829:TYR:CD2	2.53	0.43
1:A:1029:TYR:HD1	1:A:1030:VAL:HG13	1.83	0.43
1:B:795:ILE:HD12	1:B:835:VAL:HG22	2.00	0.43
1:B:986:THR:C	1:B:988:ASP:N	2.70	0.43
1:A:1017:LEU:O	1:A:1024:LEU:HA	2.18	0.43
1:B:855:ILE:N	1:B:855:ILE:CD1	2.81	0.43
1:B:848:SER:O	1:B:849:PRO:C	2.56	0.43
1:A:848:SER:HB2	2:A:219:HOH:O	2.18	0.43
1:B:767:HIS:CE1	1:B:1028:ARG:HG2	2.54	0.42
1:B:979:ASN:OD1	1:B:1000:LYS:HD3	2.18	0.42
1:B:982:LEU:HD21	1:B:1015:VAL:HG11	2.01	0.42
1:A:1011:ASP:O	1:A:1012:ASP:CB	2.67	0.42
1:A:759:ILE:O	1:A:759:ILE:HG23	2.19	0.42
1:B:986:THR:C	1:B:988:ASP:H	2.23	0.42
1:A:848:SER:O	1:A:849:PRO:C	2.57	0.42
1:A:923:ASN:ND2	1:A:927:GLU:H	2.17	0.42
1:B:890:CYS:C	1:B:892:VAL:H	2.24	0.42
1:A:837:ARG:HD3	2:A:431:HOH:O	2.19	0.41
1:A:895:VAL:O	1:A:907:LYS:HA	2.21	0.41
1:A:1023:ARG:NH1	1:B:1037:MET:CE	2.83	0.41
1:B:928:ILE:O	1:B:940:VAL:HA	2.20	0.41
1:B:942:ASN:ND2	1:B:946:GLN:CG	2.83	0.41
1:A:966:ASN:HB3	1:A:968:ASN:H	1.86	0.41
1:A:1030:VAL:HG12	2:A:184:HOH:O	2.21	0.41
1:A:788:VAL:CG1	1:A:792:ASN:HA	2.51	0.41
1:B:848:SER:O	1:B:851:HIS:ND1	2.48	0.41
1:A:1005:PHE:HE1	1:A:1020:LYS:HA	1.86	0.41
1:B:923:ASN:ND2	1:B:923:ASN:C	2.73	0.40
1:B:795:ILE:HD13	1:B:842:ILE:HG12	2.03	0.40
1:A:1031:GLN:OE1	1:A:1031:GLN:HA	2.20	0.40
1:A:942:ASN:ND2	1:A:948:LEU:HD21	2.36	0.40
1:A:866:PHE:CE1	1:A:902:GLY:HA2	2.56	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	277/286 (97%)	249 (90%)	23 (8%)	5 (2%)	13	3
1	B	280/286 (98%)	254 (91%)	21 (8%)	5 (2%)	13	3
All	All	557/572 (97%)	503 (90%)	44 (8%)	10 (2%)	13	3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	851	HIS
1	A	1012	ASP
1	B	851	HIS
1	B	925	LYS
1	A	893	MET
1	A	848	SER
1	B	979	ASN
1	A	1033	ALA
1	B	847	ARG
1	B	848	SER

### 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	242/248 (98%)	231 (96%)	11 (4%)	38	21
1	B	245/248 (99%)	236 (96%)	9 (4%)	45	30
All	All	487/496 (98%)	467 (96%)	20 (4%)	41	25

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	761	ARG
1	A	803	ARG
1	A	831	ASN
1	A	851	HIS
1	A	853	ILE
1	A	900	GLN
1	A	916	PHE
1	A	923	ASN
1	A	966	ASN
1	A	995	LEU
1	A	1011	ASP
1	B	803	ARG
1	B	828	LEU
1	B	831	ASN
1	B	853	ILE
1	B	893	MET
1	B	923	ASN
1	B	982	LEU
1	B	1017	LEU
1	B	1032	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	792	ASN
1	A	831	ASN
1	A	852	GLN
1	A	861	GLN
1	A	906	HIS
1	A	923	ASN
1	A	946	GLN
1	A	966	ASN
1	A	976	ASN
1	A	979	ASN
1	A	987	GLN
1	A	990	GLN
1	B	792	ASN
1	B	831	ASN
1	B	852	GLN
1	B	906	HIS
1	B	923	ASN
1	B	946	GLN
1	B	950	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	968	ASN
1	B	976	ASN
1	B	977	HIS
1	B	978	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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	279/286 (97%)	0.09	6 (2%) 59 67	14, 25, 42, 52	0
1	B	282/286 (98%)	0.17	11 (3%) 37 43	14, 24, 40, 73	0
All	All	561/572 (98%)	0.13	17 (3%) 48 55	14, 24, 41, 73	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1035	VAL	8.4
1	B	756	LYS	5.8
1	B	757	SER	5.4
1	B	1034	PRO	5.0
1	A	1032	LEU	4.5
1	B	758	GLN	4.5
1	B	848	SER	3.9
1	A	998	LYS	3.1
1	B	978	ASN	2.7
1	A	848	SER	2.6
1	B	1031	GLN	2.6
1	B	1036	GLY	2.6
1	A	850	THR	2.5
1	B	979	ASN	2.5
1	A	892	VAL	2.4
1	A	1037	MET	2.2
1	B	850	THR	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.