



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:35 PM UTC

PDB ID : 1Q7F / pdb_00001q7f
Title : Brain Tumor NHL domain
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Deposited on : 2003-08-18
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

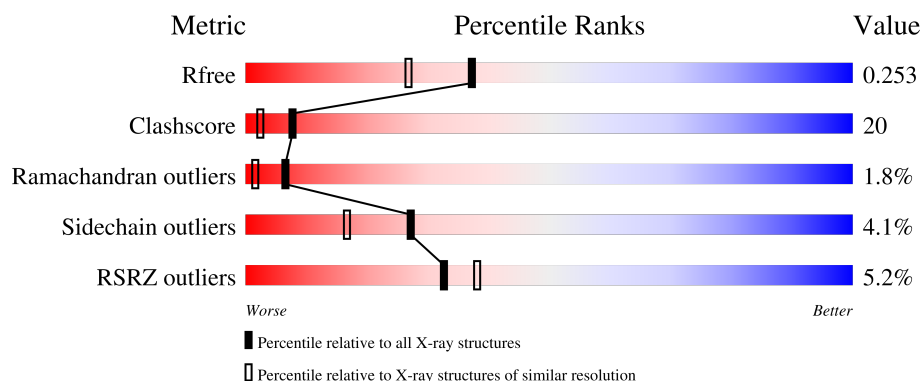
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	286	4% 68% 23% 6%
1	B	286	6% 67% 25% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5138 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 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

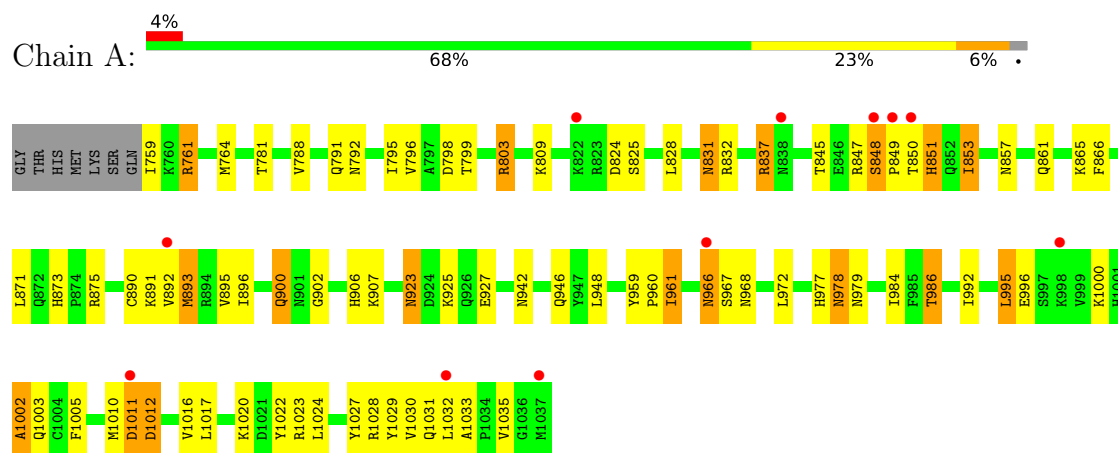
- Molecule 2 is water.

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

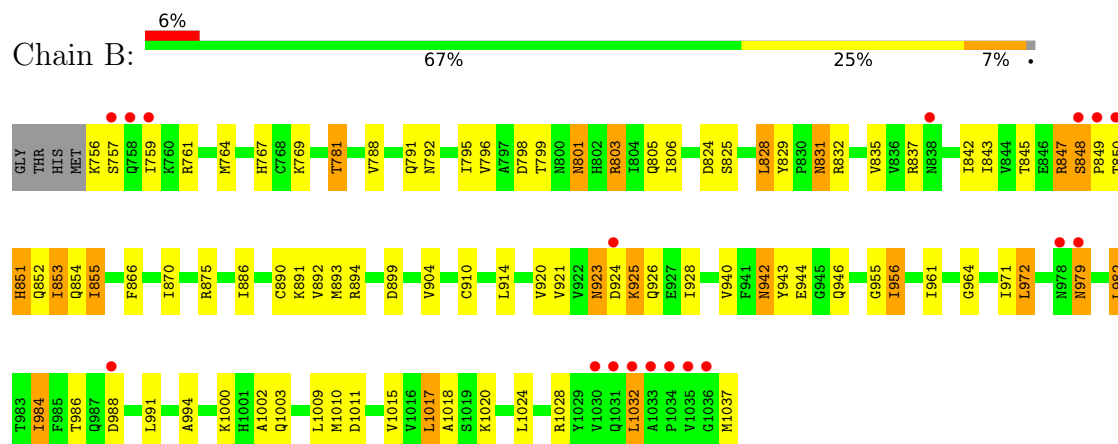
3 Residue-property plots

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

• Molecule 1: brain tumor CG10719-PA



• Molecule 1: brain tumor CG10719-PA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.77Å 94.58Å 130.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 15.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	84.6 (15.00-1.95) 84.3 (15.00-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.252 0.200 , 0.253	Depositor DCC
R_{free} test set	1425 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5138	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/2270	0.95	11/3060 (0.4%)
1	B	0.36	0/2294	0.94	11/3091 (0.4%)
All	All	0.38	0/4564	0.94	22/6151 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	781	THR	N-CA-C	-7.63	103.94	113.55
1	B	781	THR	N-CA-C	-7.26	104.40	113.55
1	A	986	THR	N-CA-C	-7.15	101.30	110.53
1	A	967	SER	N-CA-C	-7.07	103.92	112.54
1	A	978	ASN	N-CA-C	-6.96	95.98	110.80
1	A	977	HIS	N-CA-C	6.75	119.66	111.82
1	B	899	ASP	N-CA-C	-6.70	100.55	110.46
1	B	1010	MET	N-CA-C	-6.56	100.75	110.46
1	A	837	ARG	N-CA-C	6.47	118.87	111.11
1	B	801	ASN	N-CA-C	-6.22	104.97	113.30
1	B	799	THR	N-CA-C	6.21	121.56	111.37
1	A	799	THR	N-CA-C	6.18	121.50	111.37
1	B	796	VAL	N-CA-C	6.11	116.91	108.12
1	A	796	VAL	N-CA-C	5.88	117.22	108.46
1	A	1002	ALA	N-CA-C	-5.78	102.75	110.55
1	A	961	ILE	N-CA-C	-5.67	107.25	113.43
1	B	920	VAL	N-CA-C	5.53	115.14	108.06
1	B	956	ILE	CB-CA-C	-5.47	107.06	111.71
1	B	1002	ALA	N-CA-C	-5.24	103.12	110.35
1	B	942	ASN	N-CA-C	-5.24	102.71	110.46
1	B	984	ILE	N-CA-C	5.19	115.44	108.17
1	A	847	ARG	N-CA-C	5.12	116.90	110.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2227	0	2202	91	0
1	B	2251	0	2228	93	0
2	A	334	0	0	13	0
2	B	326	0	0	9	0
All	All	5138	0	4430	178	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 20.

All (178) 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:B:1032:LEU:HD12	1:B:1032:LEU:H	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:764:MET:HE2	1:A:1027:TYR:HB3	1.62	0.82
1:A:1032:LEU:O	1:A:1032:LEU:HD13	1.85	0.75
1:B:831:ASN:H	1:B:831:ASN:HD22	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:1022:TYR:HD2	1:B:1037:MET:HE2	1.54	0.73
1:B:764:MET:HE1	1:B:982:LEU:HD22	1.72	0.71
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:HD12	1:B:855:ILE:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1017:LEU:HD23	1:B:1017:LEU:C	2.23	0.63
1:B:1032:LEU:H	1:B:1032:LEU:CD1	2.00	0.63
1:A:831:ASN:O	1:A:831:ASN:ND2	2.32	0.62
1:A:986:THR:HG23	1:A:992:ILE:HD11	1.81	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:923:ASN:C	1:A:923:ASN:HD22	2.07	0.61
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:761:ARG:CZ	2:A:9:HOH:O	2.48	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:B:923:ASN:HD22	1:B:923:ASN:C	2.09	0.60
1:A:986:THR:HG22	1:A:992:ILE:HD11	1.84	0.60
1:B:854:GLN:C	1:B:855:ILE:HD12	2.26	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:1010:MET:HE2	1:A:1016:VAL:CG2	2.33	0.59
1:A:1028:ARG:NH2	1:A:1032:LEU:HB2	2.16	0.59
1:A:961:ILE:C	1:A:961:ILE:HD12	2.27	0.59
1:B:781:THR:HG23	1:B:801:ASN:ND2	2.17	0.59
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:A:890:CYS:C	1:A:892:VAL:H	2.13	0.57
1:A:795:ILE:HD12	1:A:795:ILE:N	2.20	0.57
1:B:1032:LEU:HD12	1:B:1032:LEU:N	2.05	0.57
1:A:892:VAL:HG12	1:A:892:VAL:O	2.04	0.57
1:A:848:SER:HB3	1:A:849:PRO:HD3	1.85	0.56
1:B:806:ILE:HD12	1:B:806:ILE:N	2.21	0.56
1:B:870:ILE:HD13	1:B:904:VAL:HG21	1.88	0.56
1:A:1035:VAL:HG23	2:A:653:HOH:O	2.04	0.56
1:B:824:ASP:O	1:B:825:SER:HB2	2.06	0.56
1:B:848:SER:HB3	1:B:849:PRO:HD3	1.88	0.56
1:B:942:ASN:ND2	1:B:946:GLN:HG2	2.21	0.56
1:A:824:ASP:O	1:A:825:SER:HB2	2.07	0.55
1:B:837:ARG:HH11	1:B:837:ARG:HG3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:ASN:HD22	1:B:831:ASN:N	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:B:1017:LEU:C	1:B:1017:LEU:CD2	2.80	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:1028:ARG:HG3	1:A:1028:ARG:NH1	2.23	0.53
1:A:875:ARG:HD2	2:A:437:HOH:O	2.09	0.52
1:A:1023:ARG:NH1	1:B:1037:MET:HE3	2.24	0.52
1:A:972:LEU:HD13	1:A:984:ILE:HG23	1.92	0.52
1:B:805:GLN:C	1:B:806:ILE:HD12	2.35	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:791:GLN:O	1:B:792:ASN:HB2	2.10	0.52
1:B:837:ARG:HG3	1:B:837:ARG:NH1	2.25	0.52
1:B:850:THR:O	1:B:852:GLN:N	2.43	0.52
1:B:788:VAL:CG1	1:B:792:ASN:HA	2.40	0.51
1:B:1009:LEU:HD12	1:B:1009:LEU:N	2.26	0.51
1:B:1003:GLN:CB	1:B:1020:LYS:HE3	2.39	0.51
1:A:995:LEU:HD22	1:A:995:LEU:N	2.26	0.50
1:A:1002:ALA:O	1:A:1003:GLN:C	2.53	0.50
1:B:921:VAL:HG11	1:B:964:GLY:HA2	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:A:849:PRO:HA	2:A:106:HOH:O	2.12	0.50
1:B:756:LYS:N	2:B:224:HOH:O	2.45	0.50
1:B:1018:ALA:HA	1:B:1024:LEU:HD13	1.94	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: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:961:ILE:C	1:B:961:ILE:HD12	2.37	0.48
1:A:923:ASN:C	1:A:923:ASN:ND2	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:959:TYR:N	1:A:960:PRO:CD	2.77	0.48
1:A:972:LEU:CD1	1:A:984:ILE:HG12	2.44	0.48
1:A:848:SER:O	1:A:851:HIS:CD2	2.66	0.47
1:A:1022:TYR:CD2	1:B:1037:MET:HE2	2.42	0.47
1:B:832:ARG:HB2	1:B:845:THR:OG1	2.14	0.47
1:B:769:LYS:HG2	2:B:52:HOH:O	2.14	0.47
1:B:848:SER:O	1:B:849:PRO:C	2.56	0.47
1:B:986:THR:C	1:B:988:ASP:N	2.70	0.47
1:A:1023:ARG:HH11	1:A:1023:ARG:HG3	1.79	0.47
1:A:848:SER:O	1:A:849:PRO:C	2.57	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:A:1023:ARG:HH12	1:B:1037:MET:HE3	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:890:CYS:C	1:B:892:VAL:H	2.24	0.46
1:A:798:ASP:OD2	1:A:803:ARG:HD2	2.16	0.46
1:B:1020:LYS:O	1:B:1020:LYS:HG2	2.15	0.46
1:B:986:THR:C	1:B:988:ASP:H	2.23	0.46
1:A:792:ASN:HB2	1:A:809:LYS:HE2	1.98	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
1:B:923:ASN:C	1:B:923:ASN:ND2	2.73	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1017:LEU:O	1:A:1024:LEU:HA	2.18	0.43
1:A:791:GLN:O	1:A:792:ASN:HB2	2.17	0.43
1:B:855:ILE:N	1:B:855:ILE:CD1	2.81	0.43
1:A:848:SER:HB2	2:A:219:HOH:O	2.18	0.43
1:B:971:ILE:C	1:B:972:LEU:HD23	2.44	0.42
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:759:ILE:O	1:A:759:ILE:HG23	2.19	0.42
1:A:1011:ASP:O	1:A:1012:ASP:CB	2.67	0.42
1:A:891:LYS:H	1:A:893:MET:HE1	1.84	0.42
1:A:923:ASN:ND2	1:A:927:GLU:H	2.17	0.42
1:A:892:VAL:O	1:A:893:MET:C	2.62	0.42
1:B:991:LEU:C	1:B:991:LEU:HD23	2.45	0.42
1:A:837:ARG:HD3	2:A:431:HOH:O	2.19	0.41
1:B:1017:LEU:HD23	1:B:1018:ALA:C	2.46	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:A:966:ASN:HB3	1:A:968:ASN:H	1.86	0.41
1:B:942:ASN:ND2	1:B:946:GLN:CG	2.83	0.41
1:A:788:VAL:CG1	1:A:792:ASN:HA	2.51	0.41
1:A:1030:VAL:HG12	2:A:184:HOH:O	2.21	0.41
1:A:1005:PHE:HE1	1:A:1020:LYS:HA	1.86	0.41
1:B:848:SER:O	1:B:851:HIS:ND1	2.48	0.41
1:A:865:LYS:NZ	2:A:103:HOH:O	2.49	0.40
1:A:1031:GLN:OE1	1:A:1031:GLN:HA	2.20	0.40
1:B:795:ILE:HD13	1:B:842:ILE:HG12	2.03	0.40
1:B:890:CYS:C	1:B:892:VAL:N	2.79	0.40
1:A:866:PHE:CE1	1:A:902:GLY:HA2	2.56	0.40
1:A:942:ASN:ND2	1:A:948:LEU:HD21	2.36	0.40
1:A:1010:MET:HE2	1:A:1016:VAL:HG22	2.02	0.40
1:B:757:SER:C	1:B:759:ILE:N	2.79	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%)	6	1
1	B	280/286 (98%)	254 (91%)	21 (8%)	5 (2%)	6	1
All	All	557/572 (97%)	503 (90%)	44 (8%)	10 (2%)	6	1

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%)	233 (96%)	9 (4%)	30	20
1	B	245/248 (99%)	234 (96%)	11 (4%)	24	14
All	All	487/496 (98%)	467 (96%)	20 (4%)	27	17

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	853	ILE
1	A	900	GLN
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	855	ILE
1	B	893	MET
1	B	923	ASN
1	B	972	LEU
1	B	982	LEU
1	B	1017	LEU
1	B	1032	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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	923	ASN
1	A	946	GLN
1	A	950	GLN
1	A	966	ASN
1	A	976	ASN
1	A	979	ASN
1	A	987	GLN
1	A	990	GLN
1	A	1003	GLN
1	B	792	ASN
1	B	831	ASN
1	B	858	GLN
1	B	906	HIS

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Mol	Chain	Res	Type
1	B	923	ASN
1	B	926	GLN
1	B	946	GLN
1	B	950	GLN
1	B	968	ASN
1	B	978	ASN
1	B	981	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/286 (97%)	0.08	11 (3%) 43 50	14, 25, 42, 52	0
1	B	282/286 (98%)	0.04	18 (6%) 25 29	14, 24, 40, 73	0
All	All	561/572 (98%)	0.06	29 (5%) 33 38	14, 24, 41, 73	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1035	VAL	4.7
1	B	848	SER	4.5
1	B	979	ASN	4.3
1	A	850	THR	3.7
1	B	978	ASN	3.6
1	A	892	VAL	3.4
1	A	1032	LEU	3.2
1	B	757	SER	3.2
1	A	848	SER	2.9
1	B	1034	PRO	2.8
1	B	988	ASP	2.6
1	B	1031	GLN	2.5
1	B	850	THR	2.5
1	B	924	ASP	2.4
1	B	1036	GLY	2.4
1	A	822	LYS	2.4
1	A	998	LYS	2.3
1	B	849	PRO	2.3
1	A	966	ASN	2.3
1	A	1011	ASP	2.2
1	B	838	ASN	2.2
1	B	1032	LEU	2.2
1	B	1033	ALA	2.2
1	A	1037	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1030	VAL	2.1
1	A	849	PRO	2.1
1	A	838	ASN	2.1
1	B	759	ILE	2.0
1	B	758	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.