



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:39 PM UTC

PDB ID : 1M7U / pdb_00001m7u
Title : Crystal structure of a novel DNA-binding domain from Ndt80, a transcriptional activator required for meiosis in yeast
Authors : Montano, S.P.; Cote, M.L.; Fingerman, I.; Pierce, M.; Vershon, A.K.; Georgiadis, M.M.
Deposited on : 2002-07-22
Resolution : 2.80 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

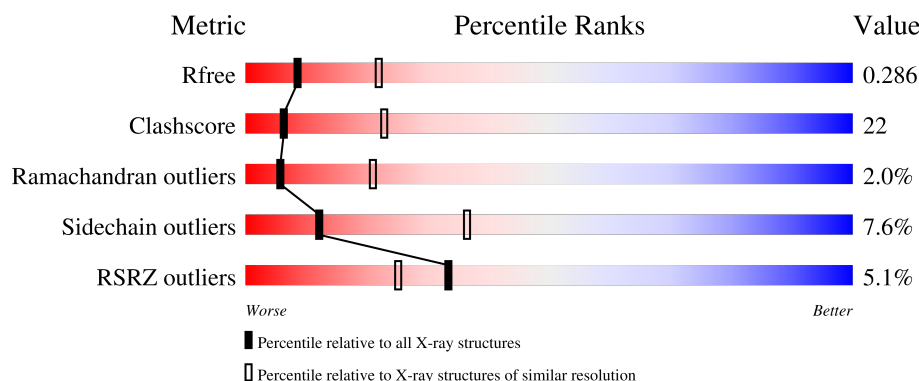
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	272	4% 56% 30% 6% 8%
1	B	272	5% 49% 34% 6% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3793 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 Ndt80 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1924	1241	319	358	6			
1	B	240	Total	C	N	O	S	0	0	0
			1823	1167	307	343	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	THR	MET	SEE REMARK 999	UNP P38830
A	225	ASN	ASP	SEE REMARK 999	UNP P38830
A	267	PHE	SER	SEE REMARK 999	UNP P38830
B	213	THR	MET	SEE REMARK 999	UNP P38830
B	225	ASN	ASP	SEE REMARK 999	UNP P38830
B	267	PHE	SER	SEE REMARK 999	UNP P38830

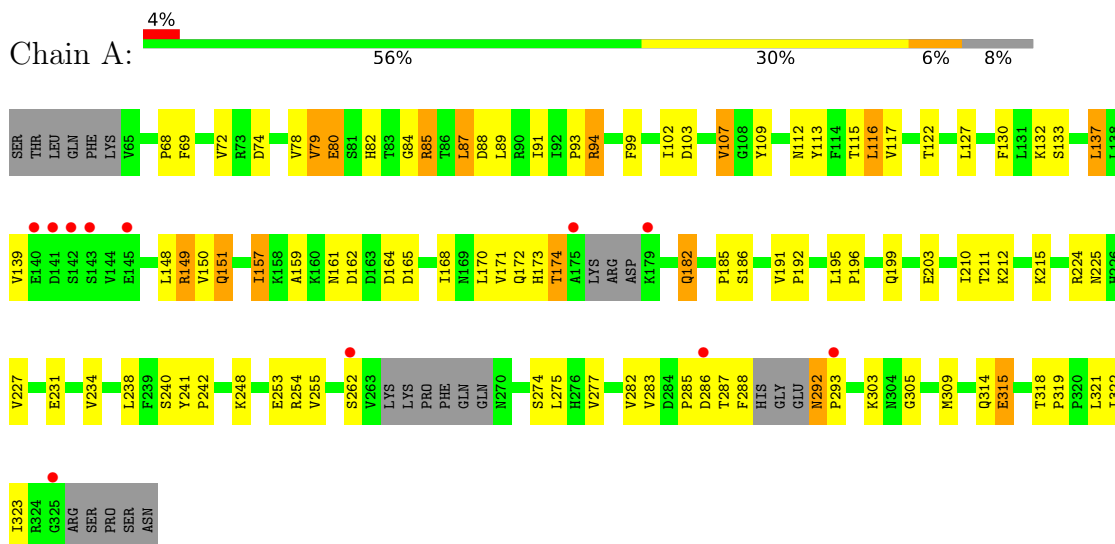
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	17	Total	O	0	0
			17	17		

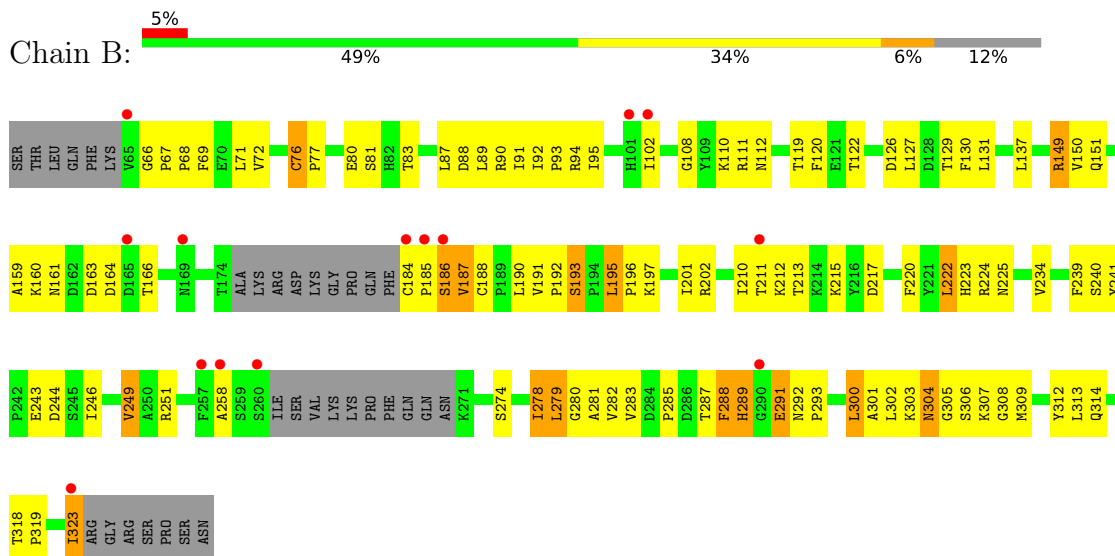
3 Residue-property plots [i](#)

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: Ndt80 protein



• Molecule 1: Ndt80 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	63.96Å 63.96Å 285.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 97.4 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.290 0.231 , 0.286	Depositor DCC
R_{free} test set	1109 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3793	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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

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	0.49	0/1972	0.98	9/2690 (0.3%)
1	B	0.49	0/1866	1.03	10/2547 (0.4%)
All	All	0.49	0/3838	1.01	19/5237 (0.4%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	LEU	N-CA-C	-7.42	98.47	110.20
1	A	107	VAL	N-CA-C	7.07	118.01	108.11
1	B	76	CYS	N-CA-C	7.07	118.56	109.65
1	B	258	ALA	N-CA-C	6.88	119.47	107.49
1	B	292	ASN	CA-C-N	6.84	126.35	119.24
1	B	292	ASN	C-N-CA	6.84	126.35	119.24
1	B	287	THR	N-CA-C	-6.67	105.18	113.38
1	B	188	CYS	N-CA-C	6.00	117.58	109.24
1	A	74	ASP	N-CA-C	-5.86	98.96	108.52
1	A	186	SER	N-CA-C	5.83	118.70	110.14
1	A	241	TYR	CA-C-N	5.77	127.05	119.84
1	A	241	TYR	C-N-CA	5.77	127.05	119.84
1	A	174	THR	N-CA-C	5.63	121.03	114.62
1	A	80	GLU	N-CA-C	-5.39	101.39	109.15
1	A	215	LYS	N-CA-C	5.36	116.81	111.07
1	B	81	SER	N-CA-C	5.23	117.66	111.33
1	A	133	SER	N-CA-C	5.12	117.44	109.60
1	B	187	VAL	N-CA-C	-5.06	100.34	107.98
1	B	108	GLY	N-CA-C	-5.03	103.91	112.51

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	1924	0	1809	77	0
1	B	1823	0	1700	89	0
2	A	29	0	0	1	0
2	B	17	0	0	0	0
All	All	3793	0	3509	161	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 22.

All (161) 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:A:211:THR:HG22	1:A:212:LYS:HE3	1.43	0.99
1:B:323:ILE:H	1:B:323:ILE:HD12	1.29	0.98
1:A:285:PRO:HA	1:A:288:PHE:CE2	2.06	0.91
1:A:72:VAL:HB	1:A:315:GLU:HG2	1.51	0.88
1:B:91:ILE:H	1:B:314:GLN:NE2	1.72	0.88
1:B:90:ARG:HA	1:B:314:GLN:HE22	1.45	0.80
1:A:285:PRO:HG3	1:A:309:MET:HE2	1.66	0.78
1:B:220:PHE:CE2	1:B:251:ARG:HD3	2.19	0.77
1:B:288:PHE:HE2	1:B:293:PRO:HA	1.50	0.76
1:B:126:ASP:OD1	1:B:129:THR:HB	1.87	0.75
1:A:149:ARG:HB2	1:A:149:ARG:HH11	1.52	0.74
1:B:288:PHE:CE2	1:B:293:PRO:HA	2.23	0.73
1:A:91:ILE:HG22	1:A:93:PRO:HG3	1.70	0.73
1:B:71:LEU:HD23	1:B:72:VAL:N	2.04	0.72
1:B:323:ILE:HD12	1:B:323:ILE:N	2.04	0.72
1:B:67:PRO:HD2	1:B:95:ILE:HD12	1.72	0.71
1:B:161:ASN:OD1	1:B:164:ASP:N	2.22	0.71
1:B:131:LEU:HD11	1:B:222:LEU:HD11	1.73	0.69
1:B:220:PHE:HE2	1:B:251:ARG:HD3	1.58	0.69
1:B:91:ILE:H	1:B:314:GLN:HE21	1.39	0.68
1:A:171:VAL:CG1	1:A:182:GLN:HG3	2.24	0.67
1:A:159:ALA:HB2	1:A:170:LEU:HD21	1.77	0.66
1:A:171:VAL:HG13	1:A:182:GLN:HG3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:HG23	1:A:253:GLU:HG2	1.80	0.64
1:B:119:THR:HG22	1:B:249:VAL:HB	1.80	0.64
1:A:292:ASN:HD22	1:A:292:ASN:N	1.96	0.62
1:B:88:ASP:O	1:B:122:THR:HA	1.99	0.62
1:A:87:LEU:HD13	1:A:89:LEU:HD21	1.81	0.62
1:A:211:THR:CG2	1:A:212:LYS:HE3	2.25	0.61
1:A:78:VAL:HG22	1:A:137:LEU:HD12	1.82	0.61
1:B:279:LEU:HD13	1:B:313:LEU:HD12	1.83	0.60
1:A:157:ILE:HD11	1:A:277:VAL:HG22	1.82	0.60
1:B:312:TYR:O	1:B:313:LEU:HD23	2.02	0.59
1:B:94:ARG:NH2	1:B:201:ILE:HG13	2.17	0.59
1:A:80:GLU:HB2	1:B:234:VAL:HG22	1.85	0.58
1:B:302:LEU:HB3	1:B:306:SER:O	2.03	0.58
1:A:162:ASP:OD2	1:A:274:SER:HB2	2.02	0.58
1:B:151:GLN:O	1:B:240:SER:OG	2.16	0.58
1:B:280:GLY:HA2	1:B:313:LEU:HG	1.85	0.58
1:B:291:GLU:O	1:B:293:PRO:HD3	2.04	0.57
1:A:91:ILE:H	1:A:314:GLN:NE2	2.02	0.57
1:A:283:VAL:HG23	1:A:309:MET:HE3	1.85	0.57
1:A:224:ARG:O	1:A:227:VAL:HG22	2.05	0.57
1:A:283:VAL:HG22	1:A:309:MET:HB2	1.86	0.57
1:B:187:VAL:HG21	1:B:300:LEU:HD12	1.85	0.57
1:A:225:ASN:H	1:A:225:ASN:HD22	1.54	0.55
1:B:278:ILE:HD11	1:B:312:TYR:CD2	2.41	0.55
1:B:195:LEU:HD23	1:B:196:PRO:HD2	1.89	0.55
1:B:288:PHE:O	1:B:289:HIS:C	2.50	0.54
1:A:172:GLN:HE21	1:A:185:PRO:HA	1.73	0.54
1:A:282:VAL:HA	1:A:309:MET:O	2.07	0.54
1:A:109:TYR:HB2	1:A:112:ASN:OD1	2.07	0.54
1:B:151:GLN:C	1:B:240:SER:HG	2.14	0.53
1:B:161:ASN:ND2	1:B:166:THR:H	2.05	0.53
1:A:195:LEU:HD13	1:A:196:PRO:O	2.09	0.53
1:A:137:LEU:HD13	1:A:150:VAL:CG2	2.40	0.52
1:B:285:PRO:HG2	1:B:307:LYS:O	2.09	0.52
1:A:303:LYS:C	1:A:305:GLY:H	2.17	0.52
1:B:302:LEU:HD23	1:B:304:ASN:N	2.25	0.52
1:B:94:ARG:HH21	1:B:201:ILE:HG13	1.73	0.52
1:B:282:VAL:HA	1:B:309:MET:O	2.09	0.52
1:A:79:VAL:HG22	1:A:84:GLY:C	2.35	0.52
1:A:132:LYS:HE2	1:A:231:GLU:O	2.10	0.52
1:A:283:VAL:CG2	1:A:309:MET:HB2	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PRO:HD2	2:A:34:HOH:O	2.08	0.52
1:B:127:LEU:O	1:B:130:PHE:HB3	2.09	0.52
1:B:243:GLU:OE2	1:B:303:LYS:HE2	2.10	0.52
1:A:283:VAL:CG2	1:A:309:MET:HE3	2.40	0.51
1:B:68:PRO:O	1:B:319:PRO:HD3	2.11	0.51
1:A:91:ILE:CG2	1:A:93:PRO:HG3	2.37	0.51
1:B:87:LEU:HD23	1:B:89:LEU:HD21	1.92	0.51
1:B:225:ASN:HD22	1:B:244:ASP:HB3	1.75	0.51
1:B:91:ILE:N	1:B:314:GLN:NE2	2.52	0.51
1:A:139:VAL:HG11	1:A:293:PRO:HB3	1.92	0.51
1:A:173:HIS:CE1	1:A:182:GLN:HB2	2.46	0.50
1:A:139:VAL:HG21	1:A:148:LEU:HG	1.92	0.50
1:A:234:VAL:HG11	1:B:289:HIS:CD2	2.46	0.50
1:A:275:LEU:O	1:A:318:THR:HG23	2.11	0.50
1:B:94:ARG:HH12	1:B:197:LYS:HA	1.75	0.50
1:A:171:VAL:HG11	1:A:182:GLN:HG3	1.93	0.50
1:A:72:VAL:CB	1:A:315:GLU:HG2	2.32	0.50
1:A:78:VAL:HG22	1:A:137:LEU:CD1	2.40	0.50
1:A:99:PHE:CE2	1:A:321:LEU:HD13	2.46	0.50
1:A:322:ILE:C	1:A:323:ILE:HD12	2.37	0.50
1:B:66:GLY:HA3	1:B:95:ILE:O	2.12	0.50
1:A:285:PRO:HG3	1:A:309:MET:CE	2.40	0.49
1:B:224:ARG:NH1	1:B:244:ASP:OD1	2.45	0.49
1:B:283:VAL:HG21	1:B:288:PHE:CE1	2.47	0.49
1:B:283:VAL:HG21	1:B:288:PHE:HE1	1.78	0.49
1:B:300:LEU:HG	1:B:301:ALA:N	2.28	0.49
1:B:91:ILE:HG22	1:B:93:PRO:HG3	1.95	0.48
1:B:303:LYS:C	1:B:305:GLY:H	2.21	0.48
1:B:184:CYS:C	1:B:186:SER:H	2.21	0.48
1:B:285:PRO:HD3	1:B:308:GLY:HA2	1.96	0.48
1:A:323:ILE:HD12	1:A:323:ILE:N	2.27	0.48
1:B:161:ASN:OD1	1:B:163:ASP:N	2.47	0.47
1:B:191:VAL:HG23	1:B:246:ILE:HG21	1.96	0.47
1:B:87:LEU:CD2	1:B:89:LEU:HD21	2.44	0.47
1:A:161:ASN:HB2	1:A:168:ILE:HD11	1.96	0.47
1:B:302:LEU:HD23	1:B:304:ASN:H	1.78	0.47
1:A:91:ILE:H	1:A:314:GLN:HE22	1.62	0.47
1:B:80:GLU:OE1	1:B:83:THR:HG23	2.15	0.47
1:B:120:PHE:O	1:B:192:PRO:HA	2.14	0.47
1:A:173:HIS:HE1	1:A:182:GLN:HB2	1.80	0.46
1:A:227:VAL:HG21	1:A:238:LEU:HD21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD23	1:B:223:HIS:N	2.29	0.46
1:A:69:PHE:CE2	1:A:318:THR:HG22	2.50	0.46
1:B:224:ARG:NH2	1:B:241:TYR:O	2.45	0.46
1:B:300:LEU:C	1:B:300:LEU:HD23	2.41	0.46
1:A:94:ARG:NH1	1:A:195:LEU:HD12	2.30	0.46
1:B:160:LYS:O	1:B:274:SER:N	2.49	0.46
1:B:318:THR:HG22	1:B:319:PRO:N	2.31	0.46
1:A:80:GLU:OE1	1:A:82:HIS:HB2	2.16	0.46
1:A:137:LEU:HD13	1:A:150:VAL:HG22	1.97	0.46
1:A:172:GLN:NE2	1:A:185:PRO:HA	2.31	0.46
1:B:213:THR:HG22	1:B:215:LYS:HB3	1.98	0.46
1:A:148:LEU:HD11	1:A:293:PRO:HG2	1.98	0.46
1:B:184:CYS:C	1:B:186:SER:N	2.74	0.46
1:A:151:GLN:O	1:A:240:SER:HB2	2.16	0.45
1:B:159:ALA:HA	1:B:274:SER:O	2.17	0.45
1:B:184:CYS:O	1:B:186:SER:N	2.50	0.45
1:A:285:PRO:HA	1:A:288:PHE:HE2	1.71	0.45
1:A:130:PHE:CE2	1:A:192:PRO:HD3	2.51	0.45
1:B:127:LEU:HD22	1:B:131:LEU:HG	1.99	0.44
1:A:68:PRO:O	1:A:319:PRO:HD3	2.18	0.44
1:A:93:PRO:O	1:A:94:ARG:HB2	2.17	0.44
1:B:71:LEU:HD23	1:B:71:LEU:C	2.42	0.44
1:B:91:ILE:HG12	1:B:279:LEU:HB2	2.00	0.44
1:A:88:ASP:O	1:A:122:THR:HA	2.17	0.44
1:A:151:GLN:O	1:A:240:SER:CB	2.66	0.43
1:B:92:ILE:HG22	1:B:195:LEU:HD12	2.00	0.43
1:B:224:ARG:HH21	1:B:241:TYR:HB2	1.82	0.43
1:A:82:HIS:ND1	1:B:149:ARG:HG2	2.33	0.43
1:B:150:VAL:HG13	1:B:281:ALA:HB1	1.99	0.43
1:B:111:ARG:C	1:B:112:ASN:HD22	2.25	0.43
1:B:119:THR:CG2	1:B:249:VAL:HB	2.48	0.42
1:B:288:PHE:CD1	1:B:309:MET:HE2	2.54	0.42
1:A:113:TYR:HB3	1:A:254:ARG:HA	2.00	0.42
1:A:199:GLN:O	1:A:203:GLU:HG3	2.19	0.42
1:B:76:CYS:HA	1:B:77:PRO:HD3	1.92	0.42
1:B:211:THR:HA	1:B:217:ASP:OD1	2.20	0.42
1:B:289:HIS:O	1:B:291:GLU:N	2.49	0.42
1:B:191:VAL:CG2	1:B:246:ILE:HG21	2.49	0.42
1:A:80:GLU:HB2	1:B:234:VAL:CG2	2.49	0.42
1:A:79:VAL:CG2	1:A:84:GLY:O	2.68	0.41
1:A:116:LEU:HD12	1:A:117:VAL:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:HA	1:B:314:GLN:NE2	2.24	0.41
1:B:210:ILE:C	1:B:212:LYS:H	2.27	0.41
1:A:285:PRO:C	1:A:287:THR:H	2.29	0.41
1:A:172:GLN:HG2	1:A:255:VAL:HG22	2.01	0.41
1:A:164:ASP:O	1:A:165:ASP:HB3	2.21	0.41
1:A:191:VAL:CG1	1:A:248:LYS:HG2	2.50	0.41
1:A:85:ARG:HG3	1:B:239:PHE:CD1	2.56	0.41
1:B:303:LYS:O	1:B:305:GLY:N	2.41	0.41
1:B:89:LEU:HD23	1:B:122:THR:HG22	2.02	0.41
1:B:318:THR:HG23	1:B:319:PRO:HD2	2.02	0.41
1:A:102:ILE:HD12	1:A:107:VAL:HG21	2.03	0.41
1:B:69:PHE:CD1	1:B:93:PRO:HB2	2.55	0.41
1:B:192:PRO:O	1:B:193:SER:HB3	2.20	0.41
1:A:157:ILE:HG23	1:A:170:LEU:CD1	2.51	0.40
1:A:91:ILE:O	1:A:93:PRO:HD3	2.22	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	227/272 (84%)	195 (86%)	29 (13%)	3 (1%)	9	31
1	B	234/272 (86%)	199 (85%)	29 (12%)	6 (3%)	4	15
All	All	461/544 (85%)	394 (86%)	58 (13%)	9 (2%)	6	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	SER
1	B	102	ILE
1	B	110	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	291	GLU
1	A	103	ASP
1	B	304	ASN
1	A	94	ARG
1	B	186	SER
1	B	185	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	203/251 (81%)	188 (93%)	15 (7%)	13	37
1	B	167/251 (66%)	154 (92%)	13 (8%)	11	35
All	All	370/502 (74%)	342 (92%)	28 (8%)	12	36

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	85	ARG
1	A	87	LEU
1	A	116	LEU
1	A	127	LEU
1	A	137	LEU
1	A	149	ARG
1	A	151	GLN
1	A	157	ILE
1	A	174	THR
1	A	182	GLN
1	A	210	ILE
1	A	286	ASP
1	A	292	ASN
1	A	315	GLU
1	B	149	ARG
1	B	190	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	193	SER
1	B	195	LEU
1	B	202	ARG
1	B	222	LEU
1	B	249	VAL
1	B	278	ILE
1	B	279	LEU
1	B	288	PHE
1	B	289	HIS
1	B	300	LEU
1	B	323	ILE

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

Mol	Chain	Res	Type
1	A	172	GLN
1	A	173	HIS
1	A	182	GLN
1	A	225	ASN
1	A	247	GLN
1	A	314	GLN
1	B	112	ASN
1	B	151	GLN
1	B	225	ASN
1	B	228	ASN
1	B	247	GLN
1	B	276	HIS
1	B	314	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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, 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	249/272 (91%)	0.02	11 (4%) 39 31	18, 35, 59, 80	0
1	B	240/272 (88%)	0.25	14 (5%) 29 22	20, 40, 71, 84	0
All	All	489/544 (89%)	0.13	25 (5%) 33 25	18, 38, 68, 84	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	ASP	5.6
1	B	323	ILE	4.6
1	B	169	ASN	4.3
1	B	184	CYS	4.0
1	B	260	SER	3.4
1	B	165	ASP	3.2
1	B	65	VAL	3.1
1	B	185	PRO	2.9
1	A	142	SER	2.8
1	B	102	ILE	2.8
1	A	262	SER	2.7
1	B	258	ALA	2.7
1	A	179	LYS	2.7
1	A	140	GLU	2.6
1	A	325	GLY	2.6
1	A	143	SER	2.5
1	A	175	ALA	2.5
1	B	186	SER	2.5
1	B	257	PHE	2.5
1	B	211	THR	2.3
1	A	286	ASP	2.2
1	B	290	GLY	2.2
1	B	101	HIS	2.1
1	A	145	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	293	PRO	2.1

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.