



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:15 AM UTC

PDB ID : 3IGF / pdb_00003igf
Title : Crystal Structure of the All4481 protein from Nostoc sp. PCC 7120, Northeast Structural Genomics Consortium Target NsR300
Authors : Forouhar, F.; Abashidze, M.; Seetharaman, J.; Mao, M.; Xiao, R.; Ciccocanti, C.; Maglaqui, M.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2009-07-27
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

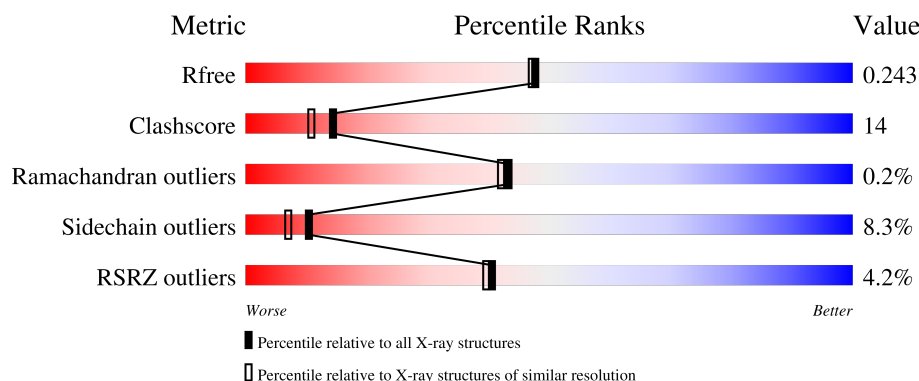
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	374	
1	B	374	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5680 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 All4481 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	Se	0	0	0
			2599	1674	439	484	2			
1	B	336	Total	C	N	O	Se	0	0	0
			2608	1676	440	490	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	THR	ALA	engineered mutation	UNP Q8YNT0
A	367	LEU	-	expression tag	UNP Q8YNT0
A	368	GLU	-	expression tag	UNP Q8YNT0
A	369	HIS	-	expression tag	UNP Q8YNT0
A	370	HIS	-	expression tag	UNP Q8YNT0
A	371	HIS	-	expression tag	UNP Q8YNT0
A	372	HIS	-	expression tag	UNP Q8YNT0
A	373	HIS	-	expression tag	UNP Q8YNT0
A	374	HIS	-	expression tag	UNP Q8YNT0
B	127	THR	ALA	engineered mutation	UNP Q8YNT0
B	367	LEU	-	expression tag	UNP Q8YNT0
B	368	GLU	-	expression tag	UNP Q8YNT0
B	369	HIS	-	expression tag	UNP Q8YNT0
B	370	HIS	-	expression tag	UNP Q8YNT0
B	371	HIS	-	expression tag	UNP Q8YNT0
B	372	HIS	-	expression tag	UNP Q8YNT0
B	373	HIS	-	expression tag	UNP Q8YNT0
B	374	HIS	-	expression tag	UNP Q8YNT0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	265	Total	O	0	0
			265	265		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	208	Total 208	O 208	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.17Å 55.55Å 122.36Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	19.96 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.2 (19.96-2.00) 95.2 (19.96-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.98Å)	Xtriage
Refinement program	CNS 1.2 & XtalView, REFMAC	Depositor
R, R_{free}	0.189 , 0.233 0.201 , 0.243	Depositor DCC
R_{free} test set	5325 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5680	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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	1.00	1/2649 (0.0%)	1.12	16/3603 (0.4%)
1	B	0.88	0/2656	1.06	11/3612 (0.3%)
All	All	0.94	1/5305 (0.0%)	1.09	27/7215 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	VAL	CA-CB	5.64	1.61	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	PRO	N-CA-C	8.42	124.38	113.86
1	B	164	LEU	N-CA-C	-7.19	104.64	113.19
1	B	33	VAL	N-CA-C	6.91	118.44	108.48
1	A	42	VAL	N-CA-C	6.61	117.40	110.72
1	A	33	VAL	N-CA-C	6.21	117.42	108.48
1	A	252	SER	N-CA-C	5.90	118.82	110.50
1	A	231	VAL	CB-CA-C	5.86	120.31	112.22
1	B	41	PRO	N-CA-C	5.83	122.14	114.27
1	A	125	TYR	N-CA-C	5.72	118.87	109.72
1	A	4	ILE	N-CA-C	-5.71	99.65	107.99
1	B	42	VAL	N-CA-C	5.46	115.66	110.53
1	B	341	ILE	N-CA-C	5.45	115.42	108.12
1	A	89	ARG	N-CA-C	-5.39	106.55	113.23
1	A	280	GLN	N-CA-C	5.39	120.08	112.75
1	A	135	ASP	N-CA-C	5.29	115.37	108.07
1	B	10	LYS	N-CA-C	5.21	119.49	113.18
1	B	222	THR	N-CA-C	-5.21	102.31	110.17
1	A	231	VAL	N-CA-CB	-5.20	102.77	110.58
1	B	232	ARG	N-CA-C	-5.14	105.76	111.36
1	B	280	GLN	CA-C-N	-5.12	113.36	119.05
1	B	280	GLN	C-N-CA	-5.12	113.36	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	LEU	N-CA-C	5.11	116.32	109.83
1	B	252	SER	N-CA-C	5.09	117.68	110.50
1	A	296	ALA	CA-C-N	5.07	125.00	119.78
1	A	296	ALA	C-N-CA	5.07	125.00	119.78
1	A	43	LEU	CA-C-N	5.03	124.64	119.05
1	A	43	LEU	C-N-CA	5.03	124.64	119.05

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	2599	0	2660	62	0
1	B	2608	0	2668	93	0
2	A	265	0	0	15	0
2	B	208	0	0	6	0
All	All	5680	0	5328	148	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 14.

All (148) 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:157:GLN:HE21	1:B:157:GLN:N	1.65	0.95
1:B:157:GLN:HE21	1:B:157:GLN:H	1.06	0.94
1:B:308:GLN:HE21	1:B:310:ARG:HH11	1.14	0.94
1:B:73:LEU:HD22	1:B:107:MSE:HE1	1.52	0.92
1:B:99:GLN:HE21	1:B:99:GLN:H	1.13	0.90
1:A:197:GLN:HA	1:A:200:ASN:HD22	1.34	0.90
1:A:99:GLN:HG3	1:B:326:TYR:CD2	2.11	0.85
1:B:43:LEU:HD22	1:B:47:LEU:HD22	1.59	0.84
1:A:255:THR:HG22	2:A:636:HOH:O	1.78	0.83
1:B:319:LYS:HD2	1:B:319:LYS:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:O	1:A:156:ARG:HB3	1.84	0.77
1:B:43:LEU:HB3	1:B:44:PRO:HD3	1.67	0.77
1:B:122:SER:HB2	1:B:124:LYS:HE2	1.66	0.76
1:B:303:ASP:HA	2:B:464:HOH:O	1.90	0.72
1:A:31:LYS:HE3	2:A:633:HOH:O	1.90	0.72
1:B:300:ILE:HD12	1:B:301:THR:N	2.05	0.71
1:A:358:GLN:HG3	2:A:622:HOH:O	1.91	0.70
1:B:73:LEU:CD2	1:B:107:MSE:HE1	2.22	0.69
1:A:114:ASN:HD21	1:A:117:ARG:HH21	1.41	0.69
1:A:310:ARG:HG2	1:A:363:ILE:HD12	1.74	0.69
1:B:311:LEU:HD12	1:B:362:LEU:HD23	1.76	0.68
1:B:45:LEU:HD23	1:B:45:LEU:O	1.95	0.67
1:A:99:GLN:HG3	1:B:326:TYR:CE2	2.29	0.67
1:B:319:LYS:HD2	1:B:319:LYS:N	2.10	0.66
1:A:254:GLN:CD	1:B:254:GLN:HE22	2.04	0.65
1:B:308:GLN:HE21	1:B:310:ARG:NH1	1.93	0.64
1:B:202:LEU:O	1:B:206:LYS:HG3	1.97	0.64
1:A:197:GLN:HA	1:A:200:ASN:ND2	2.10	0.64
1:B:58:ILE:HD11	1:B:62:LEU:HD13	1.80	0.62
1:B:44:PRO:HG3	1:B:51:LEU:HD22	1.81	0.62
1:B:300:ILE:HD12	1:B:301:THR:H	1.63	0.62
1:B:73:LEU:HD13	1:B:107:MSE:CE	2.30	0.61
1:A:298:LYS:HE3	2:A:411:HOH:O	2.01	0.61
1:A:21:ALA:CB	1:A:282:LEU:HD13	2.32	0.60
1:A:98:GLY:HA3	2:A:598:HOH:O	1.99	0.60
1:B:93:ILE:HD12	1:B:93:ILE:O	2.01	0.60
1:A:84:GLU:HA	1:A:88:LEU:HD13	1.83	0.60
1:B:45:LEU:HD23	1:B:45:LEU:C	2.27	0.59
1:B:79:GLU:OE1	1:B:82:LYS:HE2	2.02	0.59
1:A:21:ALA:HB2	1:A:282:LEU:HD13	1.84	0.59
1:A:114:ASN:ND2	1:A:117:ARG:HE	2.00	0.59
1:B:52:THR:HB	1:B:53:PRO:HD2	1.85	0.59
1:B:158:LEU:O	1:B:162:SER:HB3	2.02	0.59
1:B:359:ASN:O	1:B:360:ASN:HB2	2.02	0.59
1:A:11:SER:HB3	2:A:477:HOH:O	2.02	0.59
1:A:153:ARG:HG3	1:A:154:ARG:N	2.17	0.58
1:A:93:ILE:C	1:A:93:ILE:HD12	2.29	0.57
1:A:119:TYR:CE2	2:A:599:HOH:O	2.52	0.57
1:A:235:TRP:CZ2	1:A:266:LEU:HD22	2.39	0.57
1:A:43:LEU:HB3	1:A:44:PRO:HD3	1.87	0.57
1:B:11:SER:HB3	2:B:550:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HD13	1:B:64:VAL:HG11	1.86	0.57
1:B:73:LEU:HD13	1:B:107:MSE:HE1	1.87	0.57
1:B:140:ARG:HG3	1:B:140:ARG:HH21	1.69	0.56
1:B:97:TYR:O	1:B:100:GLU:HG2	2.04	0.56
1:A:90:THR:O	1:A:90:THR:HG23	2.06	0.56
1:B:43:LEU:CD2	1:B:47:LEU:HD22	2.33	0.55
1:B:309:VAL:CG2	1:B:364:ILE:HB	2.36	0.54
1:B:45:LEU:HD23	2:B:433:HOH:O	2.08	0.53
1:B:84:GLU:OE2	1:B:93:ILE:HG13	2.08	0.53
1:B:310:ARG:HG2	1:B:363:ILE:HG12	1.90	0.52
1:A:99:GLN:H	1:A:99:GLN:CD	2.17	0.52
1:A:65:VAL:HG11	2:A:599:HOH:O	2.09	0.52
1:A:261:ALA:HB3	2:A:399:HOH:O	2.10	0.52
1:B:255:THR:HG22	2:B:533:HOH:O	2.10	0.52
1:A:81:LYS:HD2	1:A:94:LYS:HA	1.91	0.52
1:A:114:ASN:O	1:A:118:GLU:HG3	2.10	0.52
1:A:368:GLU:HG3	1:A:369:HIS:N	2.24	0.52
1:A:114:ASN:HD22	1:A:117:ARG:HE	1.57	0.51
1:B:300:ILE:HD13	1:B:311:LEU:HD23	1.93	0.51
1:A:280:GLN:NE2	2:A:406:HOH:O	2.21	0.51
1:B:318:LYS:N	2:B:468:HOH:O	2.44	0.51
1:B:352:ILE:H	1:B:352:ILE:HD12	1.75	0.51
1:B:77:TRP:CE3	1:B:80:VAL:HG21	2.46	0.50
1:B:77:TRP:O	1:B:80:VAL:HG22	2.12	0.50
1:B:318:LYS:HD2	1:B:318:LYS:H	1.77	0.49
1:A:137:PHE:CE1	1:B:133:THR:HG21	2.48	0.49
1:B:352:ILE:HD12	1:B:352:ILE:N	2.27	0.49
1:B:163:ASP:C	1:B:165:GLY:H	2.20	0.49
1:A:96:VAL:HG23	1:B:158:LEU:HD11	1.95	0.48
1:A:67:PHE:CE1	2:A:599:HOH:O	2.56	0.48
1:A:97:TYR:CD1	1:B:326:TYR:HB3	2.49	0.48
1:B:302:ILE:HG12	1:B:309:VAL:HG12	1.96	0.48
1:A:43:LEU:N	1:A:44:PRO:CD	2.77	0.47
1:B:83:LEU:C	1:B:85:ALA:H	2.23	0.47
1:A:81:LYS:CD	1:A:94:LYS:HA	2.44	0.47
1:B:45:LEU:C	1:B:45:LEU:CD2	2.87	0.47
1:A:153:ARG:HA	1:A:156:ARG:HD2	1.97	0.47
1:B:73:LEU:HD13	1:B:107:MSE:HE3	1.96	0.47
1:B:60:PRO:O	1:B:61:ASN:HB2	2.14	0.46
1:A:219:LEU:HD13	1:A:231:VAL:HG13	1.98	0.46
1:A:273:ASP:HB3	2:A:480:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:GLU:HG3	2:B:576:HOH:O	2.16	0.46
1:B:95:GLU:O	1:B:95:GLU:HG3	2.14	0.46
1:A:346:ALA:C	1:A:347:LEU:HD12	2.40	0.46
1:B:99:GLN:HE21	1:B:99:GLN:N	1.97	0.46
1:A:67:PHE:HE1	2:A:599:HOH:O	1.95	0.45
1:A:2:ALA:N	2:A:478:HOH:O	2.49	0.45
1:A:77:TRP:CD2	1:A:101:LEU:HD11	2.51	0.45
1:B:83:LEU:C	1:B:85:ALA:N	2.75	0.45
1:B:157:GLN:N	1:B:157:GLN:NE2	2.48	0.45
1:B:43:LEU:HB3	1:B:44:PRO:CD	2.44	0.45
1:B:219:LEU:HD12	1:B:248:VAL:HG22	1.99	0.45
1:B:59:ALA:HB1	1:B:60:PRO:HD2	1.99	0.45
1:B:140:ARG:HG3	1:B:140:ARG:NH2	2.31	0.45
1:A:250:GLN:CD	1:A:259:LEU:HD22	2.42	0.44
1:B:97:TYR:HB3	1:B:99:GLN:NE2	2.32	0.44
1:A:154:ARG:HB2	1:A:154:ARG:HH21	1.82	0.44
1:B:99:GLN:H	1:B:99:GLN:NE2	1.96	0.44
1:B:73:LEU:CD1	1:B:107:MSE:HE1	2.48	0.44
1:B:73:LEU:HD21	1:B:101:LEU:HB3	1.99	0.44
1:B:163:ASP:C	1:B:165:GLY:N	2.76	0.44
1:A:6:THR:O	1:A:217:ALA:HA	2.18	0.43
1:A:88:LEU:HD12	1:A:88:LEU:N	2.33	0.43
1:A:214:ARG:HH11	1:A:214:ARG:HG3	1.83	0.43
1:B:300:ILE:HD13	1:B:311:LEU:CD2	2.48	0.43
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.91	0.43
1:B:323:LEU:CD1	1:B:332:VAL:HG22	2.49	0.43
1:A:52:THR:HB	1:A:53:PRO:CD	2.49	0.43
1:A:92:ILE:C	1:A:92:ILE:HD13	2.44	0.43
1:A:104:LEU:O	1:A:107:MSE:HB2	2.19	0.43
1:A:273:ASP:HB3	2:A:635:HOH:O	2.19	0.42
1:B:58:ILE:CD1	1:B:62:LEU:HD13	2.48	0.42
1:B:97:TYR:HB3	1:B:99:GLN:HE22	1.84	0.42
1:A:87:TYR:C	1:A:88:LEU:HD12	2.44	0.42
1:A:137:PHE:CD1	1:A:137:PHE:N	2.87	0.42
1:A:319:LYS:O	1:A:319:LYS:HD3	2.19	0.42
1:A:93:ILE:C	1:A:93:ILE:CD1	2.92	0.42
1:B:144:LEU:O	1:B:148:LEU:HG	2.19	0.42
1:B:156:ARG:HA	1:B:156:ARG:HD2	1.61	0.42
1:B:203:ASP:OD1	1:B:206:LYS:HE2	2.20	0.42
1:B:235:TRP:CZ2	1:B:266:LEU:HD22	2.55	0.42
1:B:323:LEU:HD13	1:B:332:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:CB	1:B:44:PRO:HD3	2.42	0.41
1:B:77:TRP:CZ3	1:B:80:VAL:HG21	2.56	0.41
1:A:96:VAL:HG23	1:B:158:LEU:CD1	2.50	0.41
1:B:348:SER:O	1:B:350:ARG:N	2.47	0.41
1:A:104:LEU:HD12	1:A:107:MSE:HE3	2.01	0.41
1:B:348:SER:C	1:B:350:ARG:H	2.29	0.41
1:A:290:VAL:O	1:A:294:GLU:HG3	2.21	0.41
1:A:195:THR:HA	1:A:198:VAL:CG2	2.51	0.41
1:B:6:THR:O	1:B:217:ALA:HA	2.20	0.41
1:B:222:THR:HB	1:B:253:SER:HB3	2.02	0.41
1:B:86:GLN:OE1	1:B:86:GLN:O	2.39	0.40
1:B:93:ILE:HG13	1:B:93:ILE:H	1.80	0.40
1:B:355:ALA:HA	1:B:363:ILE:O	2.22	0.40
1:B:85:ALA:C	1:B:87:TYR:H	2.29	0.40
1:B:194:PRO:O	1:B:198:VAL:HG23	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	329/374 (88%)	323 (98%)	6 (2%)	0	100	100
1	B	330/374 (88%)	316 (96%)	13 (4%)	1 (0%)	36	35
All	All	659/748 (88%)	639 (97%)	19 (3%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	349	GLY

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	282/316 (89%)	260 (92%)	22 (8%)	11	8
1	B	284/316 (90%)	259 (91%)	25 (9%)	9	6
All	All	566/632 (90%)	519 (92%)	47 (8%)	10	7

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	50	THR
1	A	62	LEU
1	A	73	LEU
1	A	81	LYS
1	A	92	ILE
1	A	99	GLN
1	A	108	ASP
1	A	154	ARG
1	A	157	GLN
1	A	231	VAL
1	A	234	LEU
1	A	255	THR
1	A	259	LEU
1	A	265	PRO
1	A	266	LEU
1	A	275	THR
1	A	276	LYS
1	A	282	LEU
1	A	317	ASP
1	A	318	LYS
1	A	319	LYS
1	B	5	LEU
1	B	11	SER
1	B	43	LEU
1	B	47	LEU
1	B	51	LEU

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Mol	Chain	Res	Type
1	B	62	LEU
1	B	86	GLN
1	B	93	ILE
1	B	99	GLN
1	B	101	LEU
1	B	146	GLU
1	B	157	GLN
1	B	234	LEU
1	B	254	GLN
1	B	255	THR
1	B	265	PRO
1	B	266	LEU
1	B	272	PRO
1	B	300	ILE
1	B	304	THR
1	B	313	LEU
1	B	319	LYS
1	B	338	ARG
1	B	356	LYS
1	B	359	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	114	ASN
1	A	157	GLN
1	A	200	ASN
1	A	295	GLN
1	A	325	GLN
1	B	56	GLN
1	B	61	ASN
1	B	86	GLN
1	B	99	GLN
1	B	157	GLN
1	B	196	ASN
1	B	200	ASN
1	B	250	GLN
1	B	254	GLN
1	B	280	GLN
1	B	292	GLN
1	B	308	GLN

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	325	GLN
1	B	360	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	331/374 (88%)	-0.24	10 (3%) 52 51	16, 27, 62, 92	0
1	B	334/374 (89%)	0.08	18 (5%) 31 30	20, 34, 75, 83	0
All	All	665/748 (88%)	-0.08	28 (4%) 40 39	16, 30, 73, 92	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	TYR	4.8
1	A	155	PHE	3.7
1	A	195	THR	3.7
1	B	345	PRO	3.6
1	B	351	PRO	3.5
1	B	353	THR	3.5
1	B	352	ILE	3.5
1	B	346	ALA	3.5
1	A	159	PHE	3.4
1	A	88	LEU	3.4
1	A	369	HIS	3.3
1	A	87	TYR	3.2
1	A	196	ASN	3.2
1	A	86	GLN	3.0
1	A	157	GLN	3.0
1	B	165	GLY	2.9
1	A	90	THR	2.8
1	B	160	VAL	2.7
1	B	347	LEU	2.6
1	B	85	ALA	2.6
1	B	365	SER	2.5
1	B	164	LEU	2.5
1	B	344	PRO	2.4
1	B	326	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	194	PRO	2.2
1	B	317	ASP	2.2
1	B	348	SER	2.2
1	B	349	GLY	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.