



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:01 PM EDT

PDB ID : 2FZ1 / pdb_00002fz1
Title : Structure of Empty Head Turnip Yellow Mosaic Virus (ATC) at 100 K
Authors : Larson, S.B.; Lucas, R.W.; McPherson, A.
Deposited on : 2006-02-08
Resolution : 2.90 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

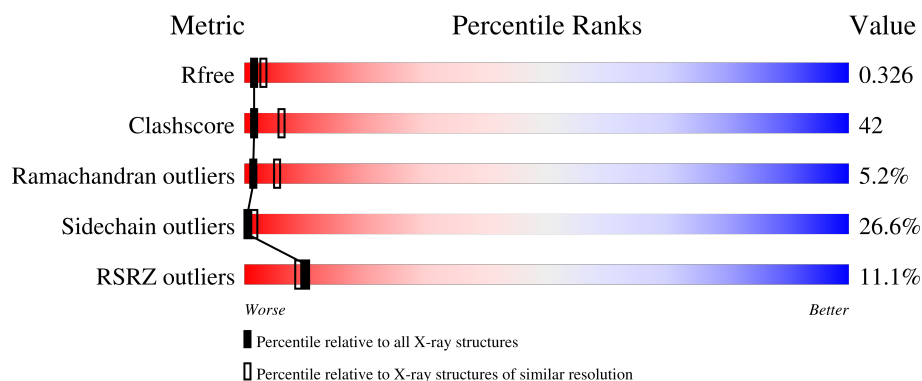
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	189	
1	B	189	
1	C	189	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4058 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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1224	787	194	236	7			
1	B	189	Total	C	N	O	S	0	0	0
			1417	909	225	275	8			
1	C	189	Total	C	N	O	S	0	0	0
			1417	909	225	275	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLN	ASN	variant	UNP P20125
A	123	GLN	ASN	variant	UNP P20125
A	138	GLN	ASN	variant	UNP P20125
B	99	GLN	ASN	variant	UNP P20125
B	123	GLN	ASN	variant	UNP P20125
B	138	GLN	ASN	variant	UNP P20125
C	99	GLN	ASN	variant	UNP P20125
C	123	GLN	ASN	variant	UNP P20125
C	138	GLN	ASN	variant	UNP P20125

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.

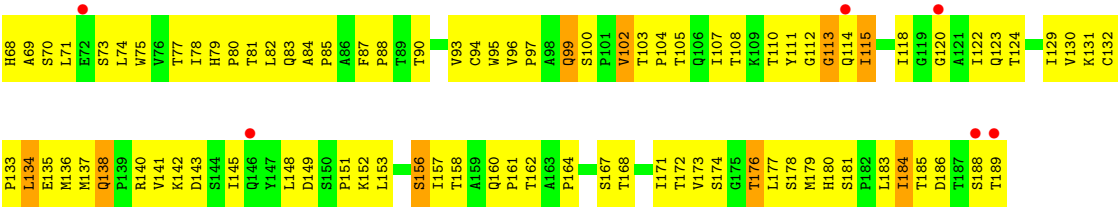
Chain A:

Amino Acid	Percentage
MET	10%
GLU	28%
ILE	28%
ASP	28%
LYS	28%
GLU	28%
LEU	28%
ALA	28%
PRO	28%
GLN	28%
ASP	28%
THR	28%
VAL	28%
THR	28%
VAL	28%
ALA	28%
THR	28%
VAL	28%
LEU	28%
PRO	28%
THR	28%
VAL	28%
PRO	28%
GLY	28%
PRO	33%
S27	33%
P28	33%
P29	33%
T30	33%
I31	33%
K32	33%
K33	33%
P34	33%
V39	33%
L40	33%
F41	33%
A42	33%
G43	33%
T44	33%
K45	33%
D46	33%
A47	33%
P48	33%
A49	33%
S50	33%
L51	33%
T52	33%
I53	33%
A54	33%
N55	33%
I56	33%
D57	33%
S58	33%
GLY	14%

Chain B:

Category	Count
M1	1
M2	1
M3	1
M4	1
M5	1
M6	1
M7	1
M8	1
M9	1
M10	1
M11	1
M12	1
M13	1
M14	1
M15	1
M16	1
M17	1
M18	1
M19	1
M20	1
M21	1
M22	1
M23	1
M24	1
M25	1
M26	1
M27	1
M28	1
M29	1
M30	1
M31	1
M32	1
M33	1
M34	1
M35	1
M36	1
M37	1

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	511.36Å 511.36Å 304.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.64 – 2.90 48.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	49.2 (48.64-2.90) 55.6 (48.64-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.48 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.309 , 0.315 0.322 , 0.326	Depositor DCC
R_{free} test set	14121 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.26	EDS
Total number of atoms	4058	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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	0.71	0/1255	1.22	14/1724 (0.8%)
1	B	0.71	0/1452	1.33	25/1997 (1.3%)
1	C	0.34	0/1452	0.94	3/1997 (0.2%)
All	All	0.61	0/4159	1.17	42/5718 (0.7%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	GLN	CA-C-N	9.28	128.93	119.56
1	B	138	GLN	C-N-CA	9.28	128.93	119.56
1	B	100	SER	CA-C-N	8.27	130.17	119.84
1	B	100	SER	C-N-CA	8.27	130.17	119.84
1	B	163	ALA	CA-C-N	7.41	128.01	120.38
1	B	163	ALA	C-N-CA	7.41	128.01	120.38
1	B	102	VAL	N-CA-C	7.29	119.49	109.80
1	B	164	PRO	CA-C-N	7.05	127.36	119.32
1	B	164	PRO	C-N-CA	7.05	127.36	119.32
1	B	40	LEU	N-CA-C	6.95	118.95	108.46
1	B	12	ARG	N-CA-C	6.83	119.32	109.14
1	A	33	GLN	CA-C-N	6.83	128.37	119.84
1	A	33	GLN	C-N-CA	6.83	128.37	119.84
1	B	53	ILE	N-CA-C	6.65	117.14	110.23
1	C	138	GLN	CA-C-N	6.63	125.87	118.97
1	C	138	GLN	C-N-CA	6.63	125.87	118.97
1	A	51	LEU	N-CA-C	6.54	119.46	108.02
1	B	129	ILE	N-CA-C	6.45	117.41	108.12
1	A	181	SER	CA-C-N	6.45	126.40	119.76
1	A	181	SER	C-N-CA	6.45	126.40	119.76
1	A	100	SER	CA-C-N	6.39	127.83	119.84
1	A	100	SER	C-N-CA	6.39	127.83	119.84
1	B	16	VAL	N-CA-C	6.21	119.20	108.90
1	B	51	LEU	N-CA-C	6.16	119.75	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ALA	N-CA-C	5.92	118.17	110.53
1	B	33	GLN	CA-C-N	5.80	127.09	119.84
1	B	33	GLN	C-N-CA	5.80	127.09	119.84
1	A	65	PHE	N-CA-C	5.76	120.00	112.92
1	B	7	LEU	N-CA-C	5.72	118.09	109.23
1	A	40	LEU	N-CA-C	5.67	117.73	108.55
1	A	135	GLU	N-CA-C	-5.53	105.80	112.54
1	A	117	CYS	N-CA-C	-5.42	101.98	110.17
1	B	126	SER	CA-C-N	5.28	125.20	119.76
1	B	126	SER	C-N-CA	5.28	125.20	119.76
1	B	135	GLU	N-CA-C	-5.26	105.55	111.28
1	A	145	ILE	N-CA-C	5.21	115.67	108.23
1	A	102	VAL	N-CA-C	5.15	116.65	109.80
1	B	145	ILE	N-CA-C	5.13	114.79	108.53
1	B	53	ILE	CB-CA-C	-5.11	105.16	111.70
1	A	87	PHE	N-CA-C	5.09	117.90	108.94
1	C	14	VAL	N-CA-C	5.07	115.58	108.89
1	B	63	THR	N-CA-C	5.04	118.53	112.38

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	1224	0	1250	113	0
1	B	1417	0	1454	128	0
1	C	1417	0	1454	121	0
All	All	4058	0	4158	347	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 42.

All (347) 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:153:LEU:HD13	1:B:155:ILE:HD11	1.30	1.06
1:B:81:THR:HG23	1:B:83:GLN:H	1.20	1.05
1:A:30:THR:HG23	1:A:180:HIS:HB3	1.34	1.03
1:B:30:THR:HG22	1:B:180:HIS:HB3	1.42	1.01
1:C:184:ILE:HD12	1:C:184:ILE:H	1.23	0.99
1:A:136:MET:HG2	1:B:184:ILE:HD11	1.43	0.98
1:C:97:PRO:HB2	1:C:99:GLN:HE22	1.32	0.94
1:C:81:THR:HG23	1:C:83:GLN:H	1.29	0.94
1:C:134:LEU:H	1:C:134:LEU:HD22	1.38	0.88
1:A:118:ILE:HA	1:A:123:GLN:HG2	1.54	0.87
1:C:10:GLN:HE22	1:C:94:CYS:HA	1.38	0.87
1:A:184:ILE:HD12	1:A:184:ILE:H	1.38	0.87
1:A:102:VAL:HG13	1:A:106:GLN:HG3	1.57	0.86
1:A:59:VAL:O	1:A:63:THR:HG23	1.76	0.84
1:A:88:PRO:HA	1:A:118:ILE:O	1.78	0.84
1:C:5:LYS:HD3	1:C:129:ILE:HD11	1.61	0.83
1:B:153:LEU:CD1	1:B:155:ILE:HD11	2.09	0.83
1:C:56:ILE:HG12	1:C:59:VAL:HG12	1.62	0.82
1:B:71:LEU:HD13	1:B:177:LEU:HD23	1.59	0.82
1:A:77:THR:HB	1:A:129:ILE:HG22	1.62	0.81
1:B:50:SER:C	1:B:51:LEU:HD12	2.04	0.81
1:B:63:THR:HA	1:B:179:MET:HE2	1.62	0.79
1:A:81:THR:HG23	1:A:83:GLN:H	1.47	0.78
1:A:126:SER:C	1:A:128:LEU:H	1.91	0.78
1:B:4:ASP:O	1:B:127:PRO:HD2	1.83	0.78
1:B:19:VAL:HG23	1:C:23:VAL:HG12	1.65	0.78
1:A:125:LEU:C	1:A:127:PRO:HD2	2.09	0.76
1:A:67:ARG:HH12	1:C:17:ALA:HB2	1.50	0.76
1:B:99:GLN:HE22	1:B:149:ASP:HB3	1.50	0.76
1:B:71:LEU:HD13	1:B:177:LEU:CD2	2.17	0.75
1:A:81:THR:HG22	1:A:168:THR:C	2.13	0.74
1:B:77:THR:HB	1:B:79:HIS:CE1	2.22	0.74
1:A:81:THR:HG22	1:A:168:THR:O	1.88	0.73
1:A:137:MET:HE2	1:A:151:PRO:HA	1.70	0.73
1:B:154:LEU:C	1:B:155:ILE:HD12	2.14	0.72
1:B:115:ILE:HD13	1:B:115:ILE:O	1.89	0.72
1:A:90:THR:HB	1:A:158:THR:HB	1.72	0.72
1:B:148:LEU:HD12	1:B:148:LEU:H	1.56	0.71
1:B:153:LEU:HD13	1:B:155:ILE:CD1	2.16	0.71
1:A:81:THR:CG2	1:A:83:GLN:HB2	2.21	0.70
1:B:30:THR:HG22	1:B:180:HIS:CB	2.20	0.70
1:B:90:THR:HB	1:B:158:THR:HB	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HD12	1:B:3:ILE:H	1.57	0.69
1:B:15:THR:HG22	1:B:136:MET:HG3	1.71	0.69
1:C:81:THR:HG21	1:C:167:SER:O	1.91	0.69
1:B:77:THR:HG23	1:B:129:ILE:HG12	1.74	0.69
1:C:97:PRO:CB	1:C:99:GLN:HE22	2.05	0.69
1:B:95:TRP:CE2	1:B:132:CYS:HB2	2.28	0.69
1:B:74:LEU:HD22	1:B:75:TRP:N	2.08	0.68
1:C:61:THR:HA	1:C:64:THR:HG23	1.76	0.68
1:A:123:GLN:HA	1:A:123:GLN:HE21	1.58	0.67
1:B:74:LEU:HD22	1:B:75:TRP:H	1.57	0.67
1:B:40:LEU:HD22	1:B:41:PHE:N	2.09	0.67
1:A:118:ILE:HA	1:A:123:GLN:CG	2.25	0.67
1:B:60:SER:O	1:B:64:THR:HG23	1.95	0.66
1:A:87:PHE:CD1	1:A:164:PRO:HB3	2.29	0.66
1:C:90:THR:HB	1:C:158:THR:HB	1.78	0.66
1:B:39:VAL:HG11	1:B:173:VAL:HG23	1.76	0.66
1:A:81:THR:HG21	1:A:167:SER:O	1.96	0.65
1:C:93:VAL:HG11	1:C:130:VAL:HG11	1.78	0.65
1:A:81:THR:HG23	1:A:83:GLN:HB2	1.78	0.65
1:B:32:LYS:HA	1:B:177:LEU:O	1.97	0.64
1:A:103:THR:O	1:A:106:GLN:HG2	1.98	0.64
1:A:39:VAL:HG22	1:A:171:ILE:O	1.98	0.64
1:B:81:THR:HG23	1:B:83:GLN:N	2.04	0.64
1:C:97:PRO:HB2	1:C:99:GLN:NE2	2.07	0.64
1:B:81:THR:HG22	1:B:168:THR:O	1.97	0.64
1:B:103:THR:HG23	1:B:106:GLN:CG	2.27	0.64
1:C:184:ILE:H	1:C:184:ILE:CD1	2.00	0.63
1:C:71:LEU:HD23	1:C:177:LEU:HB3	1.79	0.63
1:A:74:LEU:HG	1:A:75:TRP:N	2.13	0.63
1:B:102:VAL:HA	1:B:106:GLN:HE21	1.62	0.63
1:C:84:ALA:N	1:C:85:PRO:HD2	2.13	0.63
1:B:5:LYS:HD3	1:B:129:ILE:HD11	1.80	0.62
1:B:103:THR:HG23	1:B:106:GLN:CD	2.25	0.62
1:A:31:ILE:HD12	1:A:31:ILE:O	1.99	0.62
1:A:126:SER:N	1:A:127:PRO:HD2	2.15	0.62
1:A:98:ALA:HB3	1:A:148:LEU:O	2.00	0.61
1:A:61:THR:HG22	1:A:62:LEU:N	2.14	0.61
1:A:123:GLN:O	1:A:124:THR:HG23	1.99	0.61
1:C:88:PRO:HG3	1:C:120:GLY:HA3	1.82	0.61
1:A:125:LEU:HD13	1:A:127:PRO:HG3	1.82	0.61
1:B:160:GLN:HG3	1:B:161:PRO:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ILE:HG12	1:C:59:VAL:CG1	2.31	0.60
1:B:19:VAL:HG11	1:B:140:ARG:CZ	2.31	0.60
1:A:126:SER:O	1:A:128:LEU:N	2.34	0.60
1:B:99:GLN:NE2	1:B:149:ASP:HB3	2.16	0.60
1:C:56:ILE:CG1	1:C:59:VAL:HG12	2.31	0.60
1:C:107:ILE:HD12	1:C:156:SER:HB3	1.84	0.60
1:A:30:THR:HG22	1:A:179:MET:O	2.01	0.60
1:C:122:ILE:O	1:C:124:THR:HG23	2.02	0.60
1:C:160:GLN:HG3	1:C:161:PRO:HD2	1.84	0.59
1:A:184:ILE:H	1:A:184:ILE:CD1	2.14	0.59
1:A:96:VAL:C	1:A:137:MET:HE1	2.28	0.58
1:A:125:LEU:HB3	1:A:127:PRO:HD2	1.86	0.58
1:B:81:THR:HG21	1:B:167:SER:O	2.03	0.58
1:A:99:GLN:O	1:A:99:GLN:HG2	2.04	0.57
1:A:58:SER:O	1:A:62:LEU:HD12	2.05	0.57
1:A:154:LEU:N	1:A:154:LEU:HD23	2.19	0.57
1:B:146:GLN:O	1:C:145:ILE:HD13	2.04	0.57
1:A:136:MET:HG2	1:B:184:ILE:CD1	2.28	0.57
1:B:75:TRP:CB	1:B:131:LYS:HA	2.34	0.57
1:B:89:THR:OG1	1:B:168:THR:HG21	2.05	0.57
1:C:104:PRO:O	1:C:107:ILE:HG13	2.04	0.57
1:A:153:LEU:HD22	1:A:154:LEU:N	2.19	0.57
1:C:77:THR:HB	1:C:79:HIS:CE1	2.40	0.57
1:B:84:ALA:N	1:B:85:PRO:HD2	2.20	0.56
1:A:81:THR:HG23	1:A:83:GLN:N	2.20	0.56
1:B:56:ILE:O	1:B:57:ASP:C	2.48	0.56
1:B:87:PHE:CG	1:B:164:PRO:HB3	2.41	0.56
1:B:83:GLN:HA	1:B:83:GLN:NE2	2.20	0.56
1:C:87:PHE:CG	1:C:164:PRO:HB3	2.40	0.56
1:B:17:ALA:HB1	1:B:138:GLN:HG2	1.88	0.56
1:C:73:SER:OG	1:C:176:THR:HG23	2.06	0.56
1:C:77:THR:HG23	1:C:129:ILE:HG12	1.87	0.56
1:C:3:ILE:HD12	1:C:3:ILE:H	1.71	0.55
1:B:31:ILE:HD12	1:B:31:ILE:H	1.71	0.55
1:A:126:SER:N	1:A:127:PRO:CD	2.70	0.55
1:C:171:ILE:HD12	1:C:171:ILE:N	2.21	0.55
1:B:17:ALA:O	1:C:23:VAL:HG13	2.06	0.55
1:C:75:TRP:CE2	1:C:174:SER:HB2	2.42	0.55
1:B:63:THR:HA	1:B:179:MET:CE	2.36	0.55
1:B:20:LEU:HD12	1:B:20:LEU:O	2.06	0.55
1:C:3:ILE:HD12	1:C:3:ILE:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HA	1:A:177:LEU:O	2.07	0.54
1:A:103:THR:HG23	1:A:106:GLN:CD	2.32	0.54
1:C:54:ALA:HA	1:C:141:VAL:HG13	1.87	0.54
1:C:88:PRO:HA	1:C:118:ILE:O	2.07	0.54
1:A:122:ILE:HG12	1:A:122:ILE:O	2.07	0.54
1:A:95:TRP:CE2	1:A:132:CYS:HB2	2.43	0.54
1:A:49:ALA:HB3	1:A:155:ILE:HB	1.90	0.54
1:A:67:ARG:NH1	1:C:17:ALA:HB2	2.19	0.54
1:A:89:THR:OG1	1:A:168:THR:HG21	2.08	0.54
1:B:134:LEU:H	1:B:134:LEU:HD12	1.72	0.54
1:C:88:PRO:HG3	1:C:120:GLY:CA	2.37	0.54
1:B:40:LEU:HD22	1:B:41:PHE:H	1.72	0.54
1:A:84:ALA:HB3	1:A:85:PRO:HD3	1.88	0.54
1:B:19:VAL:CG2	1:C:23:VAL:HG12	2.36	0.54
1:B:59:VAL:O	1:B:60:SER:C	2.48	0.54
1:C:15:THR:HG23	1:C:15:THR:O	2.08	0.54
1:B:81:THR:CG2	1:B:83:GLN:H	2.07	0.53
1:C:184:ILE:HD12	1:C:184:ILE:N	2.07	0.53
1:C:34:PRO:O	1:C:35:PHE:HB3	2.09	0.53
1:A:40:LEU:HD12	1:A:41:PHE:H	1.72	0.53
1:A:117:CYS:O	1:A:123:GLN:HG2	2.09	0.53
1:B:96:VAL:HG13	1:B:100:SER:HB3	1.90	0.53
1:B:96:VAL:CG1	1:B:100:SER:HB3	2.39	0.53
1:B:63:THR:O	1:B:65:PHE:N	2.41	0.53
1:B:103:THR:H	1:B:106:GLN:HG3	1.74	0.53
1:C:74:LEU:HD12	1:C:75:TRP:H	1.74	0.53
1:C:7:LEU:C	1:C:7:LEU:HD22	2.33	0.53
1:C:19:VAL:HB	1:C:140:ARG:HD2	1.91	0.53
1:B:19:VAL:C	1:C:20:LEU:HD22	2.33	0.52
1:C:59:VAL:HG13	1:C:60:SER:N	2.24	0.52
1:B:1:MET:H1	1:B:1:MET:HE2	1.75	0.52
1:C:183:LEU:HD13	1:C:183:LEU:C	2.35	0.52
1:B:18:THR:HB	1:C:20:LEU:HB3	1.91	0.52
1:B:98:ALA:HB3	1:B:148:LEU:O	2.09	0.52
1:A:129:ILE:HD13	1:A:129:ILE:H	1.75	0.52
1:B:77:THR:HA	1:B:128:LEU:O	2.10	0.52
1:A:96:VAL:HG12	1:A:152:LYS:HB3	1.91	0.52
1:A:122:ILE:O	1:A:122:ILE:CG1	2.58	0.52
1:B:63:THR:C	1:B:65:PHE:H	2.18	0.52
1:C:133:PRO:HA	1:C:135:GLU:OE2	2.10	0.51
1:B:81:THR:HG22	1:B:168:THR:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:HIS:HE1	1:C:16:VAL:O	1.93	0.51
1:C:130:VAL:O	1:C:130:VAL:HG13	2.09	0.51
1:B:1:MET:HE2	1:B:1:MET:N	2.25	0.51
1:C:7:LEU:CD2	1:C:9:PRO:HD3	2.40	0.51
1:C:31:ILE:HD12	1:C:31:ILE:O	2.10	0.51
1:B:7:LEU:HD12	1:B:7:LEU:O	2.10	0.51
1:A:87:PHE:CG	1:A:164:PRO:HB3	2.45	0.51
1:A:184:ILE:HD12	1:A:184:ILE:N	2.17	0.51
1:C:134:LEU:H	1:C:134:LEU:CD2	2.17	0.51
1:B:20:LEU:HD23	1:B:145:ILE:HD13	1.93	0.51
1:B:7:LEU:HD12	1:B:7:LEU:C	2.36	0.50
1:B:109:LYS:HB3	1:C:186:ASP:OD1	2.10	0.50
1:A:95:TRP:CZ3	1:A:153:LEU:HB2	2.46	0.50
1:B:62:LEU:HB3	1:B:179:MET:HE1	1.94	0.50
1:B:40:LEU:CD2	1:B:41:PHE:H	2.23	0.50
1:B:124:THR:C	1:B:125:LEU:HD23	2.37	0.50
1:B:40:LEU:CD2	1:B:41:PHE:N	2.75	0.50
1:C:96:VAL:CA	1:C:137:MET:HE1	2.42	0.50
1:B:51:LEU:CD1	1:B:51:LEU:N	2.74	0.50
1:C:10:GLN:NE2	1:C:94:CYS:HA	2.18	0.50
1:A:33:GLN:HE21	1:A:34:PRO:HD2	1.77	0.50
1:B:51:LEU:HD12	1:B:51:LEU:N	2.23	0.50
1:B:180:HIS:HD2	1:B:181:SER:HB2	1.76	0.50
1:C:161:PRO:HG2	1:C:162:THR:H	1.77	0.50
1:A:58:SER:O	1:A:61:THR:HB	2.12	0.50
1:C:143:ASP:C	1:C:145:ILE:H	2.19	0.50
1:B:161:PRO:HG2	1:B:162:THR:H	1.76	0.50
1:C:7:LEU:HD22	1:C:9:PRO:HD3	1.93	0.50
1:C:56:ILE:O	1:C:57:ASP:C	2.55	0.50
1:C:95:TRP:CE2	1:C:132:CYS:HB2	2.47	0.50
1:A:59:VAL:O	1:A:60:SER:C	2.55	0.49
1:A:81:THR:HG21	1:A:83:GLN:HB2	1.92	0.49
1:A:153:LEU:C	1:A:154:LEU:HD23	2.36	0.49
1:B:19:VAL:HG11	1:B:140:ARG:NE	2.26	0.49
1:B:99:GLN:N	1:B:99:GLN:OE1	2.45	0.49
1:C:138:GLN:O	1:C:151:PRO:HD3	2.12	0.49
1:B:87:PHE:CD1	1:B:164:PRO:HB3	2.47	0.49
1:A:43:GLY:HA3	1:A:168:THR:HB	1.95	0.49
1:C:75:TRP:CB	1:C:131:LYS:HA	2.42	0.49
1:A:102:VAL:HG12	1:A:103:THR:N	2.26	0.49
1:B:18:THR:HG22	1:C:22:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:O	1:C:177:LEU:HD12	2.13	0.49
1:B:81:THR:CG2	1:B:168:THR:HA	2.43	0.49
1:B:102:VAL:HG12	1:B:103:THR:N	2.28	0.49
1:B:3:ILE:HD12	1:B:3:ILE:N	2.27	0.48
1:A:93:VAL:HG12	1:A:155:ILE:HG12	1.93	0.48
1:B:82:LEU:N	1:B:82:LEU:HD23	2.28	0.48
1:A:84:ALA:HB1	1:A:118:ILE:HG22	1.95	0.48
1:A:96:VAL:O	1:A:137:MET:HE1	2.14	0.48
1:B:103:THR:HG23	1:B:106:GLN:HG2	1.95	0.48
1:A:66:TYR:CD1	1:A:66:TYR:N	2.81	0.48
1:C:61:THR:HA	1:C:64:THR:CG2	2.43	0.48
1:C:40:LEU:HD12	1:C:41:PHE:H	1.78	0.48
1:C:74:LEU:HD12	1:C:75:TRP:N	2.28	0.48
1:B:13:THR:HG23	1:B:14:VAL:N	2.29	0.48
1:C:15:THR:CG2	1:C:136:MET:HB2	2.43	0.48
1:C:81:THR:HG22	1:C:168:THR:O	2.14	0.48
1:C:138:GLN:HB3	1:C:149:ASP:C	2.38	0.48
1:C:96:VAL:N	1:C:137:MET:HE1	2.29	0.48
1:C:96:VAL:O	1:C:152:LYS:HB3	2.14	0.48
1:B:31:ILE:HD12	1:B:31:ILE:O	2.14	0.47
1:C:30:THR:HB	1:C:180:HIS:HB3	1.94	0.47
1:B:75:TRP:HB3	1:B:131:LYS:HA	1.95	0.47
1:B:20:LEU:HD12	1:B:20:LEU:C	2.40	0.47
1:A:125:LEU:HD22	1:A:127:PRO:CD	2.44	0.47
1:C:68:HIS:HA	1:C:142:LYS:O	2.15	0.47
1:A:81:THR:CG2	1:A:168:THR:HA	2.44	0.47
1:C:81:THR:HG22	1:C:168:THR:HA	1.96	0.47
1:C:81:THR:CG2	1:C:83:GLN:H	2.13	0.47
1:B:187:THR:O	1:B:188:SER:C	2.58	0.47
1:B:155:ILE:HD12	1:B:155:ILE:N	2.29	0.47
1:C:59:VAL:HG13	1:C:60:SER:H	1.80	0.47
1:A:97:PRO:O	1:A:99:GLN:N	2.48	0.46
1:B:83:GLN:HA	1:B:83:GLN:HE21	1.80	0.46
1:B:115:ILE:HD13	1:B:115:ILE:H	1.80	0.46
1:A:125:LEU:CB	1:A:127:PRO:HD2	2.46	0.46
1:C:42:ALA:HB1	1:C:157:ILE:HG21	1.95	0.46
1:B:16:VAL:HG22	1:B:17:ALA:N	2.31	0.46
1:B:138:GLN:O	1:B:150:SER:HA	2.16	0.46
1:C:43:GLY:HA3	1:C:168:THR:H	1.81	0.46
1:C:149:ASP:OD2	1:C:149:ASP:N	2.46	0.46
1:A:98:ALA:HA	1:A:152:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD13	1:A:127:PRO:CG	2.45	0.46
1:A:126:SER:C	1:A:128:LEU:N	2.59	0.46
1:A:56:ILE:O	1:A:57:ASP:C	2.59	0.46
1:C:107:ILE:O	1:C:113:GLY:HA3	2.16	0.45
1:B:75:TRP:HB2	1:B:131:LYS:HA	1.98	0.45
1:C:15:THR:HG22	1:C:136:MET:HB2	1.97	0.45
1:C:81:THR:HG22	1:C:168:THR:C	2.41	0.45
1:A:32:LYS:NZ	1:A:72:GLU:HG2	2.31	0.45
1:A:102:VAL:CG1	1:A:103:THR:N	2.79	0.45
1:C:123:GLN:O	1:C:123:GLN:HG3	2.15	0.45
1:B:53:ILE:O	1:B:56:ILE:HG23	2.16	0.45
1:B:153:LEU:HD22	1:B:154:LEU:N	2.31	0.45
1:C:7:LEU:HB2	1:C:129:ILE:O	2.17	0.45
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.27	0.45
1:B:81:THR:HG21	1:B:168:THR:HA	1.98	0.45
1:A:186:ASP:OD2	1:A:186:ASP:C	2.59	0.45
1:B:50:SER:O	1:B:51:LEU:HD12	2.17	0.45
1:B:123:GLN:HG3	1:B:124:THR:N	2.31	0.44
1:C:62:LEU:H	1:C:62:LEU:HD12	1.82	0.44
1:C:138:GLN:HB2	1:C:149:ASP:CG	2.43	0.44
1:C:19:VAL:HG12	1:C:138:GLN:HE22	1.82	0.44
1:C:39:VAL:HB	1:C:171:ILE:O	2.18	0.44
1:C:39:VAL:HG23	1:C:172:THR:HA	2.00	0.44
1:C:114:GLN:O	1:C:115:ILE:HD12	2.17	0.44
1:B:15:THR:HG21	1:C:184:ILE:HD11	1.99	0.44
1:C:51:LEU:N	1:C:51:LEU:HD23	2.33	0.44
1:C:60:SER:O	1:C:64:THR:HG23	2.18	0.44
1:C:102:VAL:HG11	1:C:110:THR:OG1	2.17	0.44
1:A:116:PHE:CD1	1:A:116:PHE:N	2.85	0.43
1:A:168:THR:O	1:A:169:CYS:HB3	2.18	0.43
1:A:68:HIS:O	1:A:179:MET:HA	2.18	0.43
1:A:109:LYS:HB3	1:B:186:ASP:OD1	2.18	0.43
1:B:49:ALA:HB1	1:B:51:LEU:HD11	2.00	0.43
1:B:53:ILE:O	1:B:55:ASN:N	2.51	0.43
1:C:99:GLN:HE21	1:C:99:GLN:C	2.26	0.43
1:A:97:PRO:O	1:A:98:ALA:C	2.61	0.43
1:B:81:THR:HG23	1:B:82:LEU:N	2.33	0.43
1:A:71:LEU:HD23	1:A:176:THR:O	2.19	0.43
1:A:138:GLN:O	1:A:151:PRO:HD3	2.17	0.43
1:B:35:PHE:O	1:B:174:SER:HA	2.18	0.43
1:C:99:GLN:NE2	1:C:99:GLN:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD12	1:A:62:LEU:H	1.83	0.43
1:A:153:LEU:HD22	1:A:153:LEU:C	2.44	0.43
1:B:79:HIS:HE1	1:B:172:THR:OG1	2.01	0.43
1:C:68:HIS:HB2	1:C:180:HIS:CE1	2.54	0.43
1:C:78:ILE:O	1:C:80:PRO:HD3	2.19	0.43
1:A:138:GLN:HA	1:A:139:PRO:HD3	1.82	0.43
1:A:106:GLN:HG2	1:A:106:GLN:H	1.73	0.42
1:A:118:ILE:HD13	1:A:123:GLN:HG3	2.00	0.42
1:A:143:ASP:HB2	1:A:147:TYR:HE1	1.84	0.42
1:B:149:ASP:OD2	1:B:149:ASP:N	2.45	0.42
1:B:95:TRP:CZ3	1:B:153:LEU:HG	2.54	0.42
1:C:51:LEU:HD23	1:C:51:LEU:H	1.83	0.42
1:C:132:CYS:O	1:C:134:LEU:HD22	2.19	0.42
1:B:184:ILE:N	1:B:184:ILE:HD12	2.34	0.42
1:B:153:LEU:HD22	1:B:155:ILE:CD1	2.49	0.42
1:C:112:GLY:O	1:C:113:GLY:C	2.61	0.42
1:A:33:GLN:NE2	1:A:34:PRO:HD2	2.34	0.42
1:B:92:GLY:C	1:B:93:VAL:CG1	2.92	0.42
1:C:51:LEU:HD21	1:C:153:LEU:HB3	2.02	0.42
1:C:99:GLN:NE2	1:C:99:GLN:H	2.17	0.42
1:A:59:VAL:HG12	1:A:60:SER:N	2.35	0.42
1:B:56:ILE:O	1:B:56:ILE:HG13	2.20	0.42
1:B:63:THR:C	1:B:65:PHE:N	2.78	0.42
1:C:82:LEU:HD23	1:C:82:LEU:N	2.35	0.42
1:A:31:ILE:HD12	1:A:31:ILE:C	2.45	0.42
1:C:99:GLN:OE1	1:C:149:ASP:HB3	2.18	0.42
1:A:118:ILE:CA	1:A:123:GLN:HG2	2.36	0.42
1:B:125:LEU:HD23	1:B:125:LEU:N	2.34	0.41
1:C:135:GLU:H	1:C:135:GLU:CD	2.28	0.41
1:A:74:LEU:HD23	1:A:132:CYS:CB	2.51	0.41
1:A:81:THR:HG21	1:A:168:THR:HA	2.03	0.41
1:A:143:ASP:C	1:A:145:ILE:H	2.27	0.41
1:B:99:GLN:OE1	1:B:99:GLN:CA	2.68	0.41
1:C:183:LEU:HD13	1:C:183:LEU:O	2.20	0.41
1:A:137:MET:CE	1:A:151:PRO:HA	2.46	0.41
1:C:34:PRO:HA	1:C:176:THR:HA	2.02	0.41
1:B:115:ILE:O	1:B:115:ILE:CD1	2.66	0.41
1:B:163:ALA:HB1	1:B:164:PRO:HD2	2.01	0.41
1:C:69:ALA:HA	1:C:178:SER:O	2.21	0.41
1:A:68:HIS:HD2	1:A:143:ASP:OD1	2.04	0.41
1:A:99:GLN:N	1:A:99:GLN:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD22	1:A:127:PRO:HD3	2.01	0.41
1:B:3:ILE:N	1:B:3:ILE:CD1	2.84	0.41
1:A:53:ILE:C	1:A:55:ASN:H	2.29	0.41
1:C:87:PHE:CD1	1:C:164:PRO:HB3	2.56	0.41
1:A:68:HIS:HA	1:A:142:LYS:O	2.21	0.41
1:A:82:LEU:O	1:A:85:PRO:HD2	2.21	0.41
1:B:19:VAL:HG12	1:B:147:TYR:OH	2.20	0.41
1:C:53:ILE:O	1:C:54:ALA:C	2.63	0.41
1:C:99:GLN:HE21	1:C:100:SER:N	2.19	0.41
1:C:83:GLN:C	1:C:85:PRO:HD2	2.46	0.41
1:B:71:LEU:HD13	1:B:177:LEU:HD21	2.00	0.40
1:C:50:SER:HA	1:C:153:LEU:O	2.21	0.40
1:C:19:VAL:CG1	1:C:138:GLN:HE22	2.33	0.40
1:B:82:LEU:H	1:B:82:LEU:CD2	2.35	0.40
1:C:185:THR:OG1	1:C:186:ASP:N	2.54	0.40
1:A:53:ILE:O	1:A:55:ASN:N	2.54	0.40
1:A:54:ALA:HA	1:A:59:VAL:HG11	2.02	0.40
1:A:91:VAL:HB	1:A:157:ILE:HD12	2.03	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	161/189 (85%)	129 (80%)	23 (14%)	9 (6%)	1	4
1	B	187/189 (99%)	158 (84%)	19 (10%)	10 (5%)	1	5
1	C	187/189 (99%)	164 (88%)	14 (8%)	9 (5%)	2	7
All	All	535/567 (94%)	451 (84%)	56 (10%)	28 (5%)	1	5

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ALA
1	B	64	THR
1	B	188	SER
1	B	54	ALA
1	B	111	TYR
1	C	5	LYS
1	C	58	SER
1	C	59	VAL
1	C	64	THR
1	C	188	SER
1	A	122	ILE
1	A	124	THR
1	B	57	ASP
1	C	57	ASP
1	A	54	ALA
1	A	111	TYR
1	B	4	ASP
1	B	98	ALA
1	A	181	SER
1	A	188	SER
1	B	181	SER
1	C	111	TYR
1	C	113	GLY
1	C	181	SER
1	A	118	ILE
1	B	101	PRO
1	B	113	GLY
1	A	126	SER

5.3.2 Protein sidechains [i](#)

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	144/167 (86%)	93 (65%)	51 (35%)	0	0
1	B	167/167 (100%)	116 (70%)	51 (30%)	0	1
1	C	167/167 (100%)	142 (85%)	25 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	478/501 (95%)	351 (73%)	127 (27%)	0 1

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	30	THR
1	A	31	ILE
1	A	44	THR
1	A	45	LYS
1	A	46	ASP
1	A	57	ASP
1	A	60	SER
1	A	61	THR
1	A	62	LEU
1	A	67	ARG
1	A	72	GLU
1	A	74	LEU
1	A	77	THR
1	A	82	LEU
1	A	83	GLN
1	A	90	THR
1	A	91	VAL
1	A	96	VAL
1	A	99	GLN
1	A	103	THR
1	A	106	GLN
1	A	108	THR
1	A	110	THR
1	A	114	GLN
1	A	123	GLN
1	A	124	THR
1	A	125	LEU
1	A	128	LEU
1	A	129	ILE
1	A	131	LYS
1	A	134	LEU
1	A	136	MET
1	A	137	MET
1	A	143	ASP
1	A	145	ILE
1	A	148	LEU

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Mol	Chain	Res	Type
1	A	150	SER
1	A	153	LEU
1	A	154	LEU
1	A	162	THR
1	A	167	SER
1	A	168	THR
1	A	170	ILE
1	A	174	SER
1	A	176	THR
1	A	179	MET
1	A	184	ILE
1	A	187	THR
1	A	188	SER
1	A	189	THR
1	B	1	MET
1	B	3	ILE
1	B	13	THR
1	B	14	VAL
1	B	18	THR
1	B	19	VAL
1	B	23	VAL
1	B	29	PHE
1	B	31	ILE
1	B	39	VAL
1	B	40	LEU
1	B	44	THR
1	B	45	LYS
1	B	46	ASP
1	B	50	SER
1	B	52	THR
1	B	55	ASN
1	B	62	LEU
1	B	71	LEU
1	B	74	LEU
1	B	77	THR
1	B	93	VAL
1	B	96	VAL
1	B	99	GLN
1	B	103	THR
1	B	106	GLN
1	B	114	GLN
1	B	115	ILE

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Mol	Chain	Res	Type
1	B	122	ILE
1	B	123	GLN
1	B	124	THR
1	B	128	LEU
1	B	134	LEU
1	B	136	MET
1	B	137	MET
1	B	138	GLN
1	B	140	ARG
1	B	143	ASP
1	B	145	ILE
1	B	148	LEU
1	B	150	SER
1	B	153	LEU
1	B	154	LEU
1	B	156	SER
1	B	167	SER
1	B	168	THR
1	B	174	SER
1	B	179	MET
1	B	181	SER
1	B	183	LEU
1	B	187	THR
1	C	3	ILE
1	C	7	LEU
1	C	13	THR
1	C	14	VAL
1	C	16	VAL
1	C	23	VAL
1	C	30	THR
1	C	31	ILE
1	C	44	THR
1	C	57	ASP
1	C	70	SER
1	C	99	GLN
1	C	102	VAL
1	C	103	THR
1	C	105	THR
1	C	108	THR
1	C	115	ILE
1	C	134	LEU
1	C	148	LEU

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Mol	Chain	Res	Type
1	C	156	SER
1	C	173	VAL
1	C	176	THR
1	C	179	MET
1	C	184	ILE
1	C	189	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	55	ASN
1	A	68	HIS
1	A	106	GLN
1	A	114	GLN
1	A	123	GLN
1	A	180	HIS
1	B	36	GLN
1	B	79	HIS
1	B	83	GLN
1	B	106	GLN
1	B	180	HIS
1	C	10	GLN
1	C	33	GLN
1	C	55	ASN
1	C	99	GLN
1	C	106	GLN
1	C	114	GLN
1	C	123	GLN
1	C	138	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 [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	163/189 (86%)	0.60	18 (11%) 10 9	19, 37, 112, 177	0
1	B	189/189 (100%)	0.70	19 (10%) 12 10	20, 38, 89, 153	0
1	C	189/189 (100%)	0.74	23 (12%) 8 7	20, 38, 83, 109	0
All	All	541/567 (95%)	0.68	60 (11%) 10 9	19, 37, 96, 177	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ILE	8.7
1	B	25	GLY	7.7
1	A	27	SER	6.9
1	C	189	THR	6.8
1	B	189	THR	6.0
1	C	25	GLY	5.5
1	A	120	GLY	5.4
1	B	24	PRO	5.1
1	A	125	LEU	5.0
1	C	27	SER	4.6
1	B	1	MET	4.5
1	C	26	PRO	4.3
1	C	48	GLU	4.1
1	B	29	PHE	4.0
1	B	2	GLU	3.9
1	C	12	ARG	3.9
1	A	57	ASP	3.6
1	A	124	THR	3.5
1	C	146	GLN	3.4
1	A	48	GLU	3.2
1	B	23	VAL	3.2
1	A	126	SER	3.2
1	C	18	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	175	GLY	3.0
1	C	22	THR	3.0
1	C	2	GLU	2.9
1	A	121	ALA	2.9
1	B	22	THR	2.9
1	C	29	PHE	2.9
1	B	27	SER	2.8
1	B	26	PRO	2.8
1	B	5	LYS	2.8
1	B	45	LYS	2.8
1	C	1	MET	2.8
1	C	188	SER	2.7
1	A	146	GLN	2.6
1	B	19	VAL	2.6
1	B	4	ASP	2.6
1	C	24	PRO	2.6
1	A	29	PHE	2.5
1	A	162	THR	2.5
1	A	127	PRO	2.4
1	C	3	ILE	2.4
1	A	28	PRO	2.4
1	C	7	LEU	2.4
1	B	176	THR	2.4
1	B	72	GLU	2.3
1	C	50	SER	2.3
1	C	120	GLY	2.3
1	C	9	PRO	2.3
1	A	69	ALA	2.2
1	C	10	GLN	2.2
1	A	98	ALA	2.2
1	B	18	THR	2.2
1	B	3	ILE	2.2
1	A	123	GLN	2.1
1	C	72	GLU	2.1
1	C	114	GLN	2.1
1	A	119	GLY	2.0
1	C	19	VAL	2.0

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 [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.