



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:22 PM UTC

PDB ID : 1THU / pdb_00001thu
Title : THE STRUCTURES OF THREE CRYSTAL FORMS OF THE SWEET PROTEIN THAUMATIN
Authors : Ko, T.-P.; Day, J.; Greenwood, A.; McPherson, A.
Deposited on : 1994-06-10
Resolution : 2.60 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

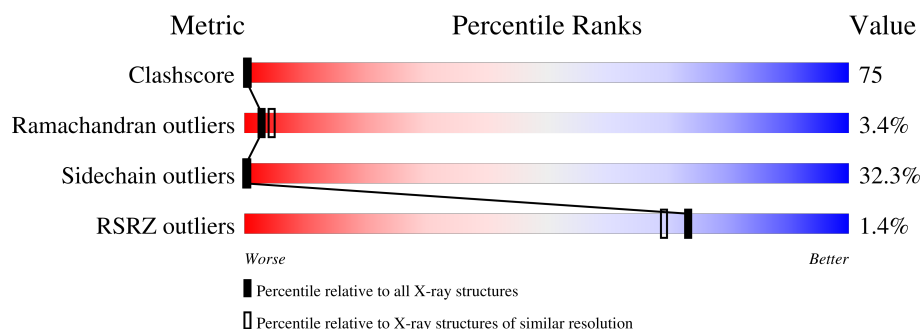
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	207	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1552 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 THAUMATIN ISOFORM B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1552	965	270	300	17			

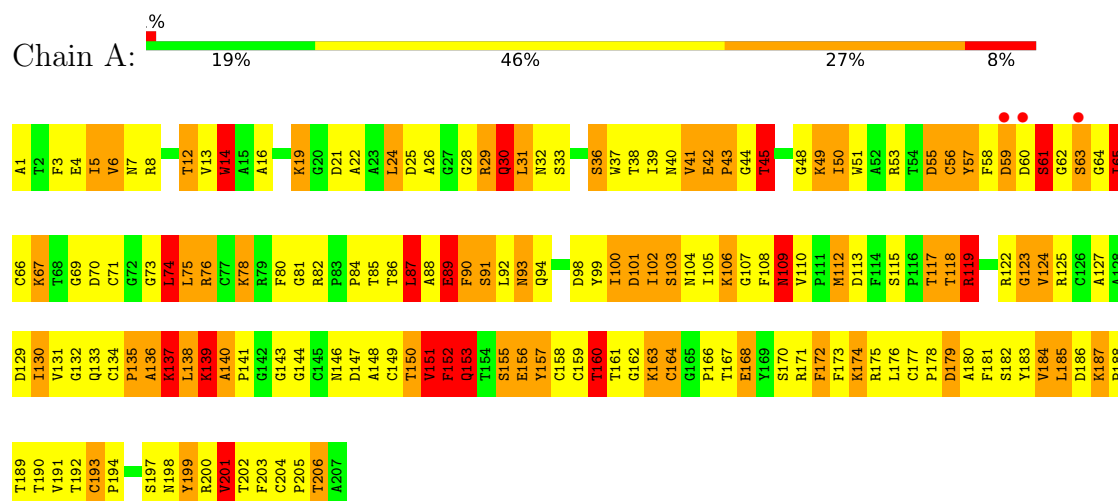
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	LYS	ASN	conflict	UNP P02883
A	113	ASP	ASN	conflict	UNP P02883

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: THAUMATIN ISOFORM B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.70Å 44.90Å 38.00Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 74.1 (8.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.54Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.184 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 152.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1552	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.19% 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	1.68	11/1588 (0.7%)	2.04	66/2150 (3.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	ASP	CG-OD1	9.09	1.42	1.25
1	A	135	PRO	N-CA	-6.98	1.39	1.47
1	A	24	LEU	CA-C	-6.95	1.44	1.52
1	A	14	TRP	CA-C	-6.35	1.44	1.53
1	A	32	ASN	C-O	5.87	1.29	1.23
1	A	29	ARG	CA-C	5.60	1.58	1.53
1	A	102	ILE	CA-C	5.55	1.59	1.52
1	A	100	ILE	CA-C	-5.36	1.46	1.52
1	A	41	VAL	N-CA	-5.35	1.39	1.46
1	A	43	PRO	N-CA	-5.09	1.41	1.47
1	A	22	ALA	C-O	-5.04	1.18	1.23

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	VAL	CB-CA-C	9.29	119.76	110.65
1	A	140	ALA	N-CA-C	8.70	120.71	109.93
1	A	63	SER	CB-CA-C	-7.25	101.69	113.37
1	A	61	SER	CA-CB-OG	-7.21	96.67	111.10
1	A	19	LYS	N-CA-C	-7.00	104.75	112.72
1	A	138	LEU	N-CA-C	-6.99	104.91	113.50
1	A	78	LYS	N-CA-C	-6.90	104.53	114.12
1	A	109	ASN	CA-CB-CG	-6.88	105.72	112.60
1	A	175	ARG	N-CA-C	-6.80	103.95	111.36
1	A	172	PHE	N-CA-C	-6.63	103.98	111.14
1	A	60	ASP	N-CA-CB	6.54	118.70	110.45
1	A	117	THR	N-CA-CB	6.51	120.12	110.49
1	A	137	LYS	N-CA-C	-6.47	105.31	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASP	N-CA-C	-6.45	104.56	112.88
1	A	22	ALA	N-CA-CB	6.41	122.52	111.69
1	A	55	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	201	VAL	N-CA-CB	6.39	118.66	110.99
1	A	152	PHE	CA-CB-CG	6.24	120.04	113.80
1	A	157	TYR	CA-C-N	-6.23	111.48	122.26
1	A	157	TYR	C-N-CA	-6.23	111.48	122.26
1	A	98	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	32	ASN	CA-CB-CG	6.10	118.70	112.60
1	A	74	LEU	N-CA-C	6.08	118.30	108.32
1	A	56	CYS	N-CA-C	6.00	118.08	109.14
1	A	87	LEU	N-CA-C	5.98	118.42	108.20
1	A	123	GLY	N-CA-C	-5.92	103.55	112.60
1	A	139	LYS	N-CA-CB	5.86	118.56	109.48
1	A	31	LEU	CA-C-N	-5.82	112.02	122.15
1	A	31	LEU	C-N-CA	-5.82	112.02	122.15
1	A	60	ASP	N-CA-C	-5.80	102.62	110.68
1	A	40	ASN	N-CA-CB	5.72	119.74	110.42
1	A	201	VAL	CA-C-N	-5.68	114.00	122.74
1	A	201	VAL	C-N-CA	-5.68	114.00	122.74
1	A	89	GLU	N-CA-C	5.65	118.69	108.69
1	A	199	TYR	N-CA-C	5.64	118.44	109.81
1	A	133	GLN	CA-C-O	5.61	126.29	119.78
1	A	42	GLU	N-CA-C	5.59	117.71	109.50
1	A	166	PRO	N-CA-CB	5.57	108.62	102.72
1	A	45	THR	CA-C-N	-5.55	115.34	123.00
1	A	45	THR	C-N-CA	-5.55	115.34	123.00
1	A	90	PHE	CA-C-N	5.54	130.58	122.77
1	A	90	PHE	C-N-CA	5.54	130.58	122.77
1	A	38	THR	N-CA-CB	5.48	119.56	110.47
1	A	139	LYS	CB-CA-C	5.45	118.01	109.84
1	A	206	THR	CA-C-N	5.43	131.48	121.70
1	A	206	THR	C-N-CA	5.43	131.48	121.70
1	A	198	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	157	TYR	O-C-N	-5.42	116.02	122.20
1	A	24	LEU	N-CA-C	-5.31	98.57	108.02
1	A	179	ASP	CB-CA-C	-5.28	99.92	110.42
1	A	30	GLN	CA-C-N	-5.27	115.03	122.94
1	A	30	GLN	C-N-CA	-5.27	115.03	122.94
1	A	153	GLN	CB-CA-C	5.23	119.80	111.48
1	A	22	ALA	N-CA-C	5.21	116.36	108.07
1	A	65	ILE	CA-C-N	5.17	131.01	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ILE	C-N-CA	5.17	131.01	122.33
1	A	78	LYS	CB-CA-C	-5.13	100.75	109.38
1	A	197	SER	O-C-N	-5.12	116.96	122.79
1	A	187	LYS	CA-C-N	5.10	126.22	119.84
1	A	187	LYS	C-N-CA	5.10	126.22	119.84
1	A	151	VAL	N-CA-C	5.09	118.52	113.53
1	A	119	ARG	CA-C-N	-5.06	111.48	121.41
1	A	119	ARG	C-N-CA	-5.06	111.48	121.41
1	A	135	PRO	CA-C-N	5.06	131.20	121.54
1	A	135	PRO	C-N-CA	5.06	131.20	121.54
1	A	19	LYS	N-CA-CB	5.04	118.21	110.70

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	1552	0	1479	228	0
All	All	1552	0	1479	228	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 75.

All (228) 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:49:LYS:HG3	1:A:89:GLU:HB3	1.31	1.11
1:A:135:PRO:HG2	1:A:138:LEU:HG	1.32	1.11
1:A:100:ILE:HG13	1:A:191:VAL:HG13	1.28	1.10
1:A:49:LYS:HB2	1:A:80:PHE:HE1	1.17	1.03
1:A:86:THR:HG22	1:A:112:MET:HE2	1.43	1.00
1:A:136:ALA:HA	1:A:139:LYS:HD2	1.48	0.96
1:A:49:LYS:HD2	1:A:80:PHE:CE1	2.01	0.95
1:A:49:LYS:HB2	1:A:80:PHE:CE1	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HD12	1:A:176:LEU:HD12	1.52	0.90
1:A:148:ALA:HB1	1:A:157:TYR:CG	2.09	0.88
1:A:108:PHE:HB3	1:A:130:ILE:HG21	1.54	0.88
1:A:55:ASP:HB3	1:A:67:LYS:HZ2	1.39	0.85
1:A:58:PHE:HA	1:A:63:SER:O	1.76	0.85
1:A:12:THR:HG22	1:A:14:TRP:CZ3	2.11	0.85
1:A:19:LYS:HB3	1:A:24:LEU:HD21	1.59	0.83
1:A:135:PRO:HG2	1:A:138:LEU:CG	2.08	0.83
1:A:55:ASP:HB3	1:A:67:LYS:NZ	1.95	0.82
1:A:148:ALA:HB1	1:A:157:TYR:CD1	2.13	0.82
1:A:100:ILE:HG13	1:A:191:VAL:CG1	2.10	0.81
1:A:62:GLY:O	1:A:74:LEU:HB3	1.80	0.81
1:A:65:ILE:CG2	1:A:66:CYS:N	2.43	0.81
1:A:56:CYS:HB2	1:A:58:PHE:CE1	2.15	0.80
1:A:109:ASN:N	1:A:109:ASN:HD22	1.78	0.80
1:A:86:THR:CG2	1:A:112:MET:HE2	2.11	0.79
1:A:29:ARG:HG3	1:A:30:GLN:H	1.46	0.79
1:A:155:SER:HA	1:A:160:THR:OG1	1.82	0.79
1:A:8:ARG:HD2	1:A:202:THR:CG2	2.13	0.79
1:A:164:CYS:HB2	1:A:185:LEU:HD12	1.63	0.78
1:A:49:LYS:CG	1:A:89:GLU:HB3	2.13	0.78
1:A:100:ILE:CG1	1:A:191:VAL:HG13	2.12	0.78
1:A:108:PHE:CB	1:A:130:ILE:HG21	2.13	0.78
1:A:109:ASN:HD22	1:A:109:ASN:H	1.30	0.77
1:A:70:ASP:O	1:A:82:ARG:HB2	1.85	0.76
1:A:86:THR:HG22	1:A:112:MET:CE	2.15	0.76
1:A:115:SER:OG	1:A:123:GLY:HA3	1.85	0.76
1:A:49:LYS:HD2	1:A:80:PHE:CZ	2.21	0.75
1:A:88:ALA:HB2	1:A:112:MET:SD	2.26	0.75
1:A:129:ASP:OD2	1:A:132:GLY:HA3	1.86	0.75
1:A:118:THR:HG22	1:A:119:ARG:H	1.51	0.73
1:A:6:VAL:HG13	1:A:36:SER:OG	1.89	0.73
1:A:129:ASP:CG	1:A:132:GLY:HA3	2.14	0.72
1:A:100:ILE:HG21	1:A:199:TYR:CE2	2.24	0.72
1:A:173:PHE:O	1:A:177:CYS:N	2.19	0.72
1:A:100:ILE:O	1:A:101:ASP:HB3	1.90	0.71
1:A:147:ASP:O	1:A:151:VAL:HG13	1.91	0.70
1:A:174:LYS:HE2	1:A:178:PRO:O	1.90	0.70
1:A:92:LEU:C	1:A:93:ASN:HD22	1.99	0.69
1:A:7:ASN:ND2	1:A:13:VAL:HG22	2.07	0.69
1:A:130:ILE:CD1	1:A:176:LEU:HD12	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:CYS:HB2	1:A:185:LEU:CD1	2.22	0.69
1:A:87:LEU:O	1:A:102:ILE:HA	1.93	0.68
1:A:8:ARG:HD2	1:A:202:THR:HG23	1.75	0.68
1:A:91:SER:C	1:A:92:LEU:HD23	2.19	0.68
1:A:65:ILE:HG23	1:A:66:CYS:N	2.08	0.68
1:A:16:ALA:HB3	1:A:51:TRP:CE2	2.30	0.67
1:A:70:ASP:HB3	1:A:82:ARG:HH11	1.59	0.67
1:A:148:ALA:CB	1:A:157:TYR:CD1	2.77	0.67
1:A:55:ASP:CB	1:A:67:LYS:NZ	2.58	0.66
1:A:185:LEU:N	1:A:185:LEU:HD23	2.08	0.66
1:A:65:ILE:HG22	1:A:66:CYS:N	2.11	0.65
1:A:127:ALA:HB2	1:A:205:PRO:HG2	1.79	0.65
1:A:67:LYS:O	1:A:82:ARG:NH2	2.27	0.64
1:A:135:PRO:HD2	1:A:138:LEU:HD12	1.80	0.64
1:A:164:CYS:CB	1:A:185:LEU:HD12	2.27	0.64
1:A:55:ASP:CB	1:A:67:LYS:HZ2	2.10	0.63
1:A:162:GLY:O	1:A:185:LEU:HD11	1.98	0.63
1:A:151:VAL:HG22	1:A:152:PHE:CD1	2.34	0.63
1:A:44:GLY:H	1:A:93:ASN:ND2	1.97	0.62
1:A:109:ASN:O	1:A:110:VAL:HG23	1.99	0.62
1:A:8:ARG:HD2	1:A:202:THR:HG21	1.81	0.62
1:A:113:ASP:O	1:A:202:THR:N	2.30	0.61
1:A:109:ASN:N	1:A:109:ASN:ND2	2.46	0.61
1:A:104:ASN:O	1:A:107:GLY:N	2.30	0.61
1:A:5:ILE:HD11	1:A:37:TRP:CE3	2.34	0.61
1:A:59:ASP:OD1	1:A:59:ASP:N	2.31	0.61
1:A:50:ILE:O	1:A:88:ALA:HB3	2.01	0.60
1:A:155:SER:HA	1:A:160:THR:HG1	1.65	0.60
1:A:163:LYS:HD3	1:A:164:CYS:N	2.16	0.60
1:A:56:CYS:CB	1:A:58:PHE:CE1	2.84	0.60
1:A:14:TRP:CD1	1:A:30:GLN:HB2	2.36	0.60
1:A:146:ASN:ND2	1:A:150:THR:HB	2.16	0.60
1:A:182:SER:OG	1:A:186:ASP:OD2	2.19	0.60
1:A:136:ALA:CA	1:A:139:LYS:HD2	2.30	0.59
1:A:146:ASN:HD21	1:A:150:THR:CG2	2.15	0.59
1:A:58:PHE:CZ	1:A:66:CYS:SG	2.96	0.59
1:A:122:ARG:HG3	1:A:191:VAL:HG21	1.85	0.58
1:A:135:PRO:CD	1:A:138:LEU:HD12	2.34	0.58
1:A:8:ARG:HH11	1:A:205:PRO:HA	1.68	0.58
1:A:184:VAL:C	1:A:186:ASP:H	2.12	0.58
1:A:155:SER:OG	1:A:156:GLU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:CG2	1:A:200:ARG:HB2	2.34	0.57
1:A:53:ARG:HH22	1:A:75:LEU:HA	1.70	0.57
1:A:56:CYS:HB3	1:A:65:ILE:O	2.05	0.57
1:A:151:VAL:HG22	1:A:152:PHE:CE1	2.40	0.56
1:A:56:CYS:CB	1:A:58:PHE:CZ	2.88	0.56
1:A:58:PHE:CA	1:A:63:SER:O	2.53	0.56
1:A:19:LYS:O	1:A:19:LYS:HG3	2.05	0.55
1:A:63:SER:OG	1:A:64:GLY:N	2.30	0.55
1:A:69:GLY:HA2	1:A:82:ARG:O	2.06	0.55
1:A:4:GLU:HG2	1:A:6:VAL:HG22	1.88	0.55
1:A:73:GLY:C	1:A:74:LEU:HG	2.31	0.55
1:A:140:ALA:HB3	1:A:144:GLY:O	2.07	0.55
1:A:147:ASP:OD2	1:A:150:THR:OG1	2.25	0.54
1:A:103:SER:HB2	1:A:181:PHE:HB2	1.88	0.54
1:A:58:PHE:HB3	1:A:63:SER:O	2.08	0.54
1:A:148:ALA:CB	1:A:157:TYR:HB3	2.37	0.54
1:A:5:ILE:HG12	1:A:37:TRP:O	2.08	0.54
1:A:14:TRP:NE1	1:A:30:GLN:HB2	2.22	0.54
1:A:161:THR:OG1	1:A:162:GLY:N	2.41	0.54
1:A:90:PHE:HA	1:A:99:TYR:O	2.08	0.53
1:A:71:CYS:O	1:A:71:CYS:SG	2.67	0.53
1:A:29:ARG:HB2	1:A:37:TRP:CE3	2.44	0.52
1:A:134:CYS:SG	1:A:138:LEU:HB2	2.50	0.52
1:A:127:ALA:HB2	1:A:205:PRO:CG	2.39	0.52
1:A:148:ALA:HB1	1:A:157:TYR:HB3	1.91	0.52
1:A:28:GLY:HA3	1:A:75:LEU:O	2.09	0.52
1:A:146:ASN:HB3	1:A:151:VAL:HG12	1.91	0.52
1:A:56:CYS:SG	1:A:58:PHE:CZ	3.03	0.52
1:A:62:GLY:O	1:A:74:LEU:CB	2.55	0.52
1:A:84:PRO:O	1:A:85:THR:HG22	2.10	0.52
1:A:148:ALA:HB1	1:A:157:TYR:CB	2.39	0.52
1:A:108:PHE:CG	1:A:130:ILE:HG21	2.45	0.52
1:A:174:LYS:HG3	1:A:182:SER:OG	2.10	0.52
1:A:90:PHE:CD1	1:A:90:PHE:N	2.78	0.51
1:A:105:ILE:HD11	1:A:183:TYR:O	2.10	0.51
1:A:149:CYS:C	1:A:151:VAL:H	2.18	0.51
1:A:159:CYS:SG	1:A:184:VAL:HG23	2.50	0.51
1:A:8:ARG:CD	1:A:202:THR:HG21	2.40	0.51
1:A:146:ASN:HB3	1:A:151:VAL:CG1	2.40	0.51
1:A:59:ASP:OD2	1:A:61:SER:HB3	2.11	0.51
1:A:4:GLU:HG2	1:A:6:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ALA:CB	1:A:205:PRO:HG2	2.40	0.50
1:A:12:THR:CG2	1:A:13:VAL:N	2.74	0.50
1:A:84:PRO:C	1:A:85:THR:CG2	2.84	0.50
1:A:84:PRO:HB3	1:A:146:ASN:OD1	2.11	0.50
1:A:151:VAL:CG2	1:A:152:PHE:CE1	2.94	0.50
1:A:13:VAL:C	1:A:14:TRP:CE3	2.90	0.50
1:A:159:CYS:C	1:A:161:THR:H	2.20	0.50
1:A:151:VAL:CG2	1:A:152:PHE:CD1	2.95	0.50
1:A:58:PHE:HZ	1:A:66:CYS:SG	2.35	0.49
1:A:5:ILE:CG2	1:A:50:ILE:CD1	2.89	0.49
1:A:12:THR:CG2	1:A:14:TRP:CZ3	2.92	0.49
1:A:58:PHE:CB	1:A:63:SER:O	2.61	0.48
1:A:109:ASN:H	1:A:109:ASN:ND2	2.07	0.48
1:A:65:ILE:HG23	1:A:66:CYS:H	1.77	0.48
1:A:66:CYS:HB2	1:A:70:ASP:HB2	1.95	0.48
1:A:93:ASN:ND2	1:A:93:ASN:N	2.61	0.48
1:A:5:ILE:CD1	1:A:37:TRP:CE3	2.96	0.48
1:A:140:ALA:HB3	1:A:144:GLY:H	1.77	0.48
1:A:92:LEU:C	1:A:93:ASN:ND2	2.69	0.47
1:A:57:TYR:O	1:A:64:GLY:HA3	2.14	0.47
1:A:155:SER:O	1:A:158:CYS:N	2.47	0.47
1:A:124:VAL:HG12	1:A:179:ASP:HB3	1.96	0.47
1:A:146:ASN:ND2	1:A:150:THR:CG2	2.77	0.47
1:A:193:CYS:HB3	1:A:194:PRO:HD2	1.97	0.47
1:A:56:CYS:SG	1:A:58:PHE:HZ	2.37	0.47
1:A:137:LYS:HB2	1:A:137:LYS:HE3	1.51	0.47
1:A:164:CYS:HB2	1:A:185:LEU:CG	2.45	0.47
1:A:14:TRP:HD1	1:A:75:LEU:CD2	2.27	0.47
1:A:42:GLU:HA	1:A:43:PRO:HD3	1.77	0.47
1:A:117:THR:HG21	1:A:200:ARG:HB2	1.96	0.47
1:A:74:LEU:O	1:A:75:LEU:C	2.58	0.46
1:A:149:CYS:C	1:A:151:VAL:N	2.74	0.46
1:A:151:VAL:C	1:A:152:PHE:HD1	2.24	0.46
1:A:70:ASP:H	1:A:82:ARG:NH1	2.13	0.46
1:A:14:TRP:HD1	1:A:75:LEU:HD21	1.81	0.46
1:A:92:LEU:O	1:A:94:GLN:NE2	2.43	0.46
1:A:5:ILE:HG21	1:A:50:ILE:HD13	1.98	0.46
1:A:37:TRP:CE2	1:A:39:ILE:HG22	2.50	0.46
1:A:87:LEU:O	1:A:103:SER:N	2.45	0.45
1:A:151:VAL:HG22	1:A:152:PHE:HD1	1.79	0.45
1:A:24:LEU:HD11	1:A:48:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASP:H	1:A:82:ARG:HH11	1.64	0.45
1:A:118:THR:HG22	1:A:119:ARG:N	2.25	0.45
1:A:81:GLY:O	1:A:106:LYS:NZ	2.49	0.45
1:A:113:ASP:O	1:A:201:VAL:HA	2.16	0.45
1:A:186:ASP:O	1:A:188:PRO:N	2.50	0.44
1:A:3:PHE:CD1	1:A:3:PHE:N	2.85	0.44
1:A:55:ASP:CB	1:A:67:LYS:HZ3	2.31	0.44
1:A:25:ASP:CG	1:A:26:ALA:N	2.74	0.44
1:A:135:PRO:O	1:A:138:LEU:N	2.35	0.44
1:A:14:TRP:N	1:A:14:TRP:HE3	2.15	0.44
1:A:170:SER:O	1:A:182:SER:HB2	2.16	0.44
1:A:187:LYS:HG2	1:A:188:PRO:HD2	1.99	0.44
1:A:14:TRP:CE3	1:A:14:TRP:N	2.85	0.44
1:A:69:GLY:HA2	1:A:85:THR:HG21	1.99	0.44
1:A:8:ARG:CD	1:A:202:THR:CG2	2.89	0.43
1:A:140:ALA:HA	1:A:141:PRO:HD2	1.74	0.43
1:A:92:LEU:HD23	1:A:92:LEU:N	2.31	0.43
1:A:108:PHE:CD1	1:A:108:PHE:C	2.96	0.43
1:A:136:ALA:HA	1:A:139:LYS:CD	2.33	0.43
1:A:42:GLU:O	1:A:45:THR:HB	2.19	0.43
1:A:112:MET:HA	1:A:202:THR:O	2.18	0.43
1:A:163:LYS:HD3	1:A:164:CYS:O	2.19	0.43
1:A:167:THR:O	1:A:168:GLU:C	2.58	0.43
1:A:26:ALA:O	1:A:76:ARG:HG2	2.19	0.43
1:A:192:THR:O	1:A:192:THR:HG22	2.18	0.43
1:A:163:LYS:HD3	1:A:163:LYS:C	2.43	0.43
1:A:193:CYS:HB3	1:A:194:PRO:CD	2.48	0.43
1:A:84:PRO:C	1:A:85:THR:HG23	2.44	0.43
1:A:181:PHE:CZ	1:A:188:PRO:HA	2.54	0.42
1:A:19:LYS:HA	1:A:48:GLY:HA2	2.01	0.42
1:A:184:VAL:C	1:A:186:ASP:N	2.77	0.42
1:A:19:LYS:HB3	1:A:24:LEU:CD2	2.41	0.42
1:A:67:LYS:C	1:A:82:ARG:HH22	2.22	0.42
1:A:104:ASN:C	1:A:106:LYS:N	2.78	0.42
1:A:140:ALA:CB	1:A:144:GLY:C	2.93	0.42
1:A:5:ILE:HG21	1:A:5:ILE:HD12	1.80	0.42
1:A:25:ASP:OD2	1:A:39:ILE:HG22	2.20	0.42
1:A:37:TRP:CE2	1:A:39:ILE:CG2	3.03	0.42
1:A:29:ARG:CG	1:A:30:GLN:H	2.22	0.41
1:A:151:VAL:C	1:A:152:PHE:CD1	2.98	0.41
1:A:14:TRP:HB3	1:A:29:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:CD1	1:A:57:TYR:N	2.88	0.41
1:A:203:PHE:O	1:A:204:CYS:HB2	2.20	0.41
1:A:70:ASP:HB3	1:A:82:ARG:NH1	2.31	0.41
1:A:174:LYS:HE3	1:A:180:ALA:O	2.19	0.41
1:A:1:ALA:O	1:A:41:VAL:N	2.44	0.41
1:A:16:ALA:HB3	1:A:51:TRP:CD2	2.55	0.41
1:A:41:VAL:HG11	1:A:90:PHE:HE2	1.85	0.41
1:A:100:ILE:O	1:A:101:ASP:CB	2.63	0.41
1:A:199:TYR:N	1:A:199:TYR:CD1	2.88	0.41
1:A:153:GLN:HA	1:A:158:CYS:SG	2.61	0.40
1:A:163:LYS:C	1:A:163:LYS:CD	2.94	0.40
1:A:49:LYS:HG3	1:A:49:LYS:HZ2	1.78	0.40
1:A:69:GLY:CA	1:A:85:THR:HG21	2.52	0.40
1:A:183:TYR:O	1:A:186:ASP:HB2	2.22	0.40
1:A:84:PRO:O	1:A:85:THR:CG2	2.70	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	205/207 (99%)	165 (80%)	33 (16%)	7 (3%)	3 4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ALA
1	A	160	THR
1	A	156	GLU
1	A	61	SER
1	A	185	LEU
1	A	193	CYS

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Mol	Chain	Res	Type
1	A	143	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	167/167 (100%)	113 (68%)	54 (32%)	0 0

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	VAL
1	A	12	THR
1	A	14	TRP
1	A	30	GLN
1	A	31	LEU
1	A	33	SER
1	A	36	SER
1	A	45	THR
1	A	49	LYS
1	A	50	ILE
1	A	57	TYR
1	A	59	ASP
1	A	61	SER
1	A	65	ILE
1	A	67	LYS
1	A	74	LEU
1	A	75	LEU
1	A	76	ARG
1	A	78	LYS
1	A	87	LEU
1	A	89	GLU
1	A	91	SER
1	A	93	ASN
1	A	101	ASP

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Mol	Chain	Res	Type
1	A	103	SER
1	A	106	LYS
1	A	109	ASN
1	A	112	MET
1	A	118	THR
1	A	119	ARG
1	A	124	VAL
1	A	125	ARG
1	A	130	ILE
1	A	131	VAL
1	A	137	LYS
1	A	139	LYS
1	A	150	THR
1	A	151	VAL
1	A	152	PHE
1	A	153	GLN
1	A	155	SER
1	A	160	THR
1	A	163	LYS
1	A	164	CYS
1	A	168	GLU
1	A	171	ARG
1	A	172	PHE
1	A	174	LYS
1	A	184	VAL
1	A	189	THR
1	A	190	THR
1	A	201	VAL
1	A	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	104	ASN
1	A	109	ASN
1	A	146	ASN

5.3.3 RNA ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	207/207 (100%)	-0.49	3 (1%) 73 69	4, 17, 28, 34	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	ASP	3.9
1	A	63	SER	3.1
1	A	59	ASP	2.5

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.