



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:44 AM UTC

PDB ID : 3Q5W / pdb_00003q5w
Title : Structure of proteasome tether
Authors : Schumacher, M.A.
Deposited on : 2010-12-30
Resolution : 2.75 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)
Validation Pipeline (wwPDB-VP) : 2.49

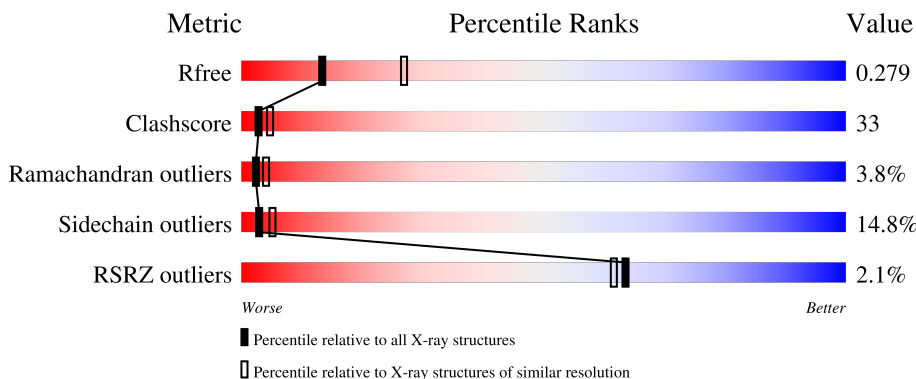
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	245	2% 34% 35% 11% • 19%
1	B	245	% 38% 33% 9% • 19%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3239 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 Protein cut8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	Se	0	0	0
			1606	1024	278	296	4	4			
1	B	199	Total	C	N	O	S	Se	0	0	0
			1620	1033	280	299	4	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP P38937
A	-18	GLY	-	expression tag	UNP P38937
A	-17	SER	-	expression tag	UNP P38937
A	-16	SER	-	expression tag	UNP P38937
A	-15	HIS	-	expression tag	UNP P38937
A	-14	HIS	-	expression tag	UNP P38937
A	-13	HIS	-	expression tag	UNP P38937
A	-12	HIS	-	expression tag	UNP P38937
A	-11	HIS	-	expression tag	UNP P38937
A	-10	HIS	-	expression tag	UNP P38937
A	-9	SER	-	expression tag	UNP P38937
A	-8	SER	-	expression tag	UNP P38937
A	-7	GLY	-	expression tag	UNP P38937
A	-6	LEU	-	expression tag	UNP P38937
A	-5	VAL	-	expression tag	UNP P38937
A	-4	PRO	-	expression tag	UNP P38937
A	-3	ARG	-	expression tag	UNP P38937
A	-2	GLY	-	expression tag	UNP P38937
A	-1	SER	-	expression tag	UNP P38937
A	0	HIS	-	expression tag	UNP P38937
B	-19	MSE	-	expression tag	UNP P38937
B	-18	GLY	-	expression tag	UNP P38937
B	-17	SER	-	expression tag	UNP P38937
B	-16	SER	-	expression tag	UNP P38937
B	-15	HIS	-	expression tag	UNP P38937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P38937
B	-13	HIS	-	expression tag	UNP P38937
B	-12	HIS	-	expression tag	UNP P38937
B	-11	HIS	-	expression tag	UNP P38937
B	-10	HIS	-	expression tag	UNP P38937
B	-9	SER	-	expression tag	UNP P38937
B	-8	SER	-	expression tag	UNP P38937
B	-7	GLY	-	expression tag	UNP P38937
B	-6	LEU	-	expression tag	UNP P38937
B	-5	VAL	-	expression tag	UNP P38937
B	-4	PRO	-	expression tag	UNP P38937
B	-3	ARG	-	expression tag	UNP P38937
B	-2	GLY	-	expression tag	UNP P38937
B	-1	SER	-	expression tag	UNP P38937
B	0	HIS	-	expression tag	UNP P38937

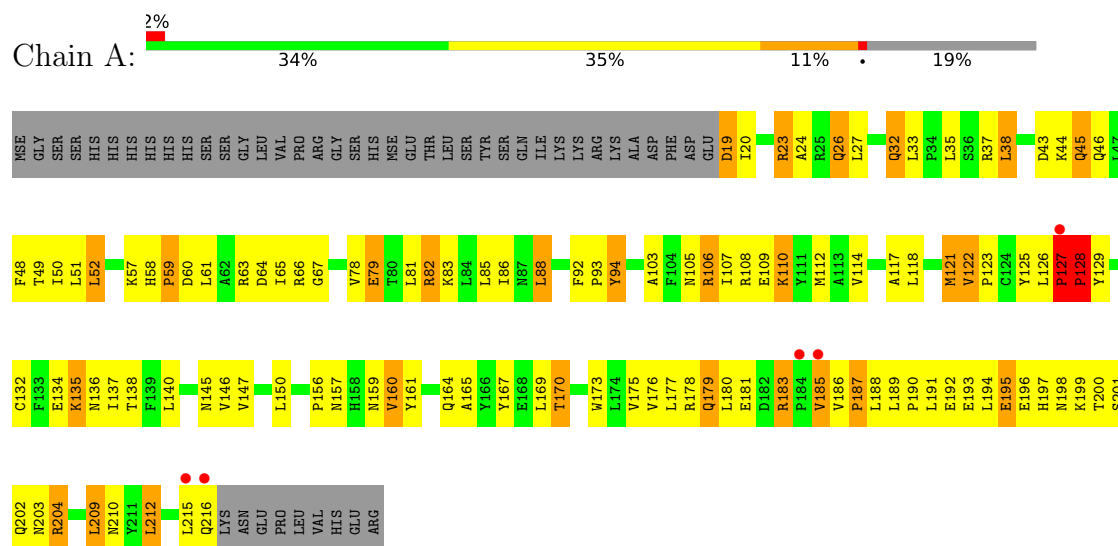
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	4	Total O 4 4	0	0

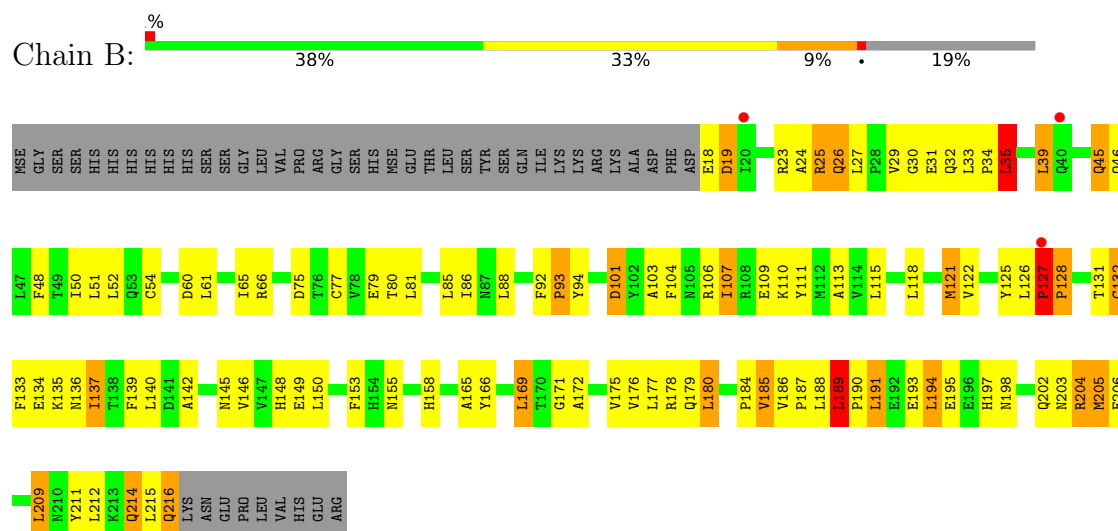
3 Residue-property plots

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: Protein cut8



• Molecule 1: Protein cut8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.66Å 51.18Å 71.33Å 103.92° 100.02° 98.00°	Depositor
Resolution (Å)	67.60 – 2.75 67.60 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.8 (67.60-2.75) 95.9 (67.60-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.231 , 0.276 0.235 , 0.279	Depositor DCC
R_{free} test set	1039 reflections (8.83%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3239	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.58% 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	0.56	1/1639 (0.1%)	1.19	12/2221 (0.5%)
1	B	0.61	0/1653	1.14	13/2239 (0.6%)
All	All	0.59	1/3292 (0.0%)	1.17	25/4460 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	VAL	CA-CB	5.28	1.56	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	CA-N-CD	-28.21	72.50	112.00
1	B	126	LEU	CA-C-N	10.91	131.62	120.38
1	B	126	LEU	C-N-CA	10.91	131.62	120.38
1	B	128	PRO	CA-N-CD	-9.91	98.12	112.00
1	B	121	MSE	N-CA-C	8.65	120.33	111.07
1	A	121	MSE	N-CA-C	8.03	120.03	111.28
1	B	127	PRO	N-CA-C	7.26	119.56	110.70
1	B	127	PRO	CA-N-CD	-6.65	102.69	112.00
1	B	19	ASP	CA-C-N	-6.40	112.18	121.65
1	B	19	ASP	C-N-CA	-6.40	112.18	121.65
1	A	58	HIS	CA-C-N	6.10	127.46	119.84
1	A	58	HIS	C-N-CA	6.10	127.46	119.84
1	A	20	ILE	N-CA-C	5.92	118.49	111.09
1	A	128	PRO	CA-CB-CG	-5.91	93.28	104.50
1	A	183	ARG	CA-C-N	5.91	125.92	119.89
1	A	183	ARG	C-N-CA	5.91	125.92	119.89
1	B	189	LEU	CA-C-N	5.85	127.16	119.84
1	B	189	LEU	C-N-CA	5.85	127.16	119.84
1	A	127	PRO	CA-C-N	5.73	127.00	119.84
1	A	127	PRO	C-N-CA	5.73	127.00	119.84
1	A	160	VAL	CB-CA-C	-5.31	104.97	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	PRO	N-CA-CB	-5.20	98.04	103.08
1	B	35	LEU	N-CA-C	5.17	116.92	111.28
1	A	170	THR	N-CA-C	-5.15	105.56	111.07
1	B	127	PRO	CB-CA-C	5.05	117.08	110.92

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	1606	0	1595	111	2
1	B	1620	0	1613	113	1
2	A	9	0	0	1	0
2	B	4	0	0	0	0
All	All	3239	0	3208	211	2

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 33.

All (211) 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:127:PRO:CG	1:B:175:VAL:HG12	1.65	1.26
1:B:127:PRO:HG2	1:B:175:VAL:HG12	1.21	1.12
1:B:127:PRO:HG2	1:B:175:VAL:CG1	1.80	1.11
1:B:33:LEU:HD12	1:B:34:PRO:HD2	1.32	1.11
1:B:77:CYS:HB3	1:B:121:MSE:HE3	1.19	1.09
1:B:189:LEU:HD22	1:B:189:LEU:H	1.24	1.02
1:B:127:PRO:HG3	1:B:175:VAL:HG12	1.48	0.94
1:A:117:ALA:HB1	1:A:121:MSE:HE3	1.53	0.90
1:A:27:LEU:HD22	1:B:178:ARG:HH21	1.36	0.87
1:B:198:ASN:HD22	1:B:209:LEU:HD12	1.38	0.87
1:A:27:LEU:HD22	1:B:178:ARG:NH2	1.91	0.85
1:A:85:LEU:HD23	1:A:146:VAL:HG13	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD11	1:B:176:VAL:HG21	1.61	0.82
1:A:110:LYS:H	1:A:110:LYS:HD2	1.45	0.81
1:A:82:ARG:HD2	1:A:82:ARG:N	1.94	0.80
1:B:107:ILE:HD12	1:B:107:ILE:N	1.97	0.80
1:B:92:PHE:HA	1:B:107:ILE:HD11	1.64	0.79
1:B:103:ALA:O	1:B:107:ILE:HD13	1.84	0.78
1:A:82:ARG:HD2	1:A:82:ARG:H	1.50	0.77
1:B:166:TYR:CD2	1:B:205:MSE:HE1	2.19	0.77
1:B:204:ARG:HG2	1:B:204:ARG:HH11	1.52	0.75
1:A:27:LEU:CD2	1:B:178:ARG:HH21	2.01	0.74
1:A:106:ARG:HH11	1:A:106:ARG:HB3	1.53	0.72
1:B:109:GLU:H	1:B:109:GLU:CD	1.97	0.71
1:A:88:LEU:HD12	1:A:107:ILE:CG2	2.21	0.71
1:B:77:CYS:CB	1:B:121:MSE:HE3	2.11	0.71
1:A:129:TYR:HB2	1:B:30:GLY:O	1.91	0.70
1:B:189:LEU:H	1:B:189:LEU:CD2	2.01	0.70
1:A:194:LEU:HB3	1:A:209:LEU:HG	1.74	0.68
1:A:114:VAL:O	1:A:118:LEU:HD23	1.93	0.68
1:A:145:ASN:ND2	1:A:197:HIS:HE1	1.91	0.68
1:A:88:LEU:HD12	1:A:107:ILE:HG22	1.75	0.68
1:B:184:PRO:O	1:B:185:VAL:HB	1.94	0.68
1:B:198:ASN:ND2	1:B:209:LEU:HD12	2.08	0.67
1:A:27:LEU:HD23	1:B:175:VAL:HG22	1.74	0.67
1:B:176:VAL:O	1:B:179:GLN:HG2	1.95	0.67
1:A:57:LYS:NZ	1:B:60:ASP:OD2	2.24	0.67
1:A:117:ALA:HB1	1:A:121:MSE:CE	2.23	0.67
1:B:198:ASN:OD1	1:B:203:ASN:HA	1.94	0.66
1:A:45:GLN:C	1:A:45:GLN:HE21	2.03	0.66
1:A:137:ILE:HG21	1:A:190:PRO:HG2	1.76	0.66
1:A:19:ASP:N	1:A:23:ARG:HH22	1.94	0.66
1:B:46:GLN:HE21	1:B:50:ILE:HD11	1.60	0.66
1:B:190:PRO:HB3	1:B:193:GLU:OE1	1.95	0.66
1:A:110:LYS:HD2	1:A:110:LYS:N	2.11	0.65
1:A:108:ARG:O	1:A:112:MSE:HG2	1.97	0.65
1:A:109:GLU:CD	1:A:109:GLU:H	2.04	0.65
1:B:107:ILE:N	1:B:107:ILE:CD1	2.59	0.65
1:A:198:ASN:OD1	1:A:203:ASN:HA	1.96	0.65
1:A:140:LEU:HD11	1:A:176:VAL:HG21	1.78	0.64
1:B:204:ARG:HH11	1:B:204:ARG:CG	2.11	0.64
1:A:145:ASN:HD21	1:A:197:HIS:HE1	1.45	0.64
1:B:172:ALA:O	1:B:176:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ALA:O	1:B:25:ARG:C	2.40	0.64
1:A:175:VAL:HG12	1:A:178:ARG:NH2	2.13	0.64
1:B:93:PRO:HB3	1:B:106:ARG:HD2	1.80	0.63
1:A:201:SER:O	1:A:204:ARG:HD2	1.97	0.63
1:A:185:VAL:HG12	1:A:186:VAL:H	1.64	0.63
1:B:26:GLN:CD	1:B:26:GLN:H	2.03	0.63
1:B:127:PRO:HB2	1:B:128:PRO:HD2	1.79	0.63
1:A:175:VAL:HG12	1:A:178:ARG:HH21	1.63	0.63
1:A:199:LYS:HD2	1:A:199:LYS:C	2.24	0.62
1:A:51:LEU:HD23	1:A:51:LEU:O	1.99	0.62
1:A:132:CYS:SG	1:A:135:LYS:HD2	2.40	0.61
1:B:46:GLN:O	1:B:50:ILE:HG13	2.00	0.61
1:B:145:ASN:HA	1:B:148:HIS:CD2	2.35	0.61
1:A:180:LEU:HD11	1:A:187:PRO:CD	2.30	0.61
1:A:147:VAL:HA	1:A:150:LEU:HD13	1.82	0.60
1:A:185:VAL:HG12	1:A:186:VAL:N	2.16	0.60
1:B:127:PRO:HG2	1:B:175:VAL:HG11	1.77	0.60
1:B:33:LEU:HD12	1:B:34:PRO:CD	2.21	0.60
1:A:45:GLN:O	1:A:48:PHE:HB3	2.01	0.60
1:B:85:LEU:HD23	1:B:146:VAL:HG13	1.84	0.60
1:A:199:LYS:HD2	1:A:200:THR:N	2.16	0.60
1:B:111:TYR:CE1	1:B:150:LEU:HD22	2.36	0.60
1:A:126:LEU:HB2	1:B:30:GLY:HA3	1.84	0.59
1:A:51:LEU:HD23	1:A:51:LEU:C	2.27	0.59
1:B:191:LEU:HD22	1:B:195:GLU:OE1	2.02	0.59
1:B:189:LEU:HB3	1:B:212:LEU:HD21	1.83	0.59
1:A:180:LEU:HD11	1:A:187:PRO:HD2	1.84	0.58
1:A:92:PHE:CD1	1:A:107:ILE:HD13	2.38	0.58
1:B:142:ALA:O	1:B:146:VAL:HG23	2.03	0.58
1:A:48:PHE:O	1:A:52:LEU:HD23	2.04	0.58
1:A:85:LEU:HD12	1:A:86:ILE:N	2.19	0.57
1:A:88:LEU:CD1	1:A:107:ILE:HG22	2.34	0.57
1:A:126:LEU:HB2	1:B:30:GLY:CA	2.34	0.57
1:B:25:ARG:HG3	1:B:25:ARG:O	2.04	0.57
1:A:81:LEU:HD21	1:A:118:LEU:HD22	1.86	0.57
1:B:177:LEU:O	1:B:180:LEU:HB2	2.05	0.57
1:B:180:LEU:HD21	1:B:189:LEU:HD11	1.85	0.56
1:A:122:VAL:N	1:A:123:PRO:HD2	2.21	0.56
1:A:33:LEU:HD12	1:A:37:ARG:HG3	1.88	0.55
1:A:191:LEU:O	1:A:191:LEU:HD23	2.05	0.55
1:B:155:ASN:HB3	1:B:158:HIS:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD12	1:B:39:LEU:HD22	1.89	0.55
1:A:60:ASP:O	1:A:63:ARG:HG2	2.07	0.55
1:B:184:PRO:O	1:B:185:VAL:CB	2.55	0.55
1:B:140:LEU:HD11	1:B:176:VAL:CG2	2.36	0.54
1:A:63:ARG:HG3	1:A:64:ASP:N	2.22	0.54
1:B:189:LEU:HD22	1:B:189:LEU:N	2.09	0.54
1:A:103:ALA:O	1:A:107:ILE:HG13	2.08	0.53
1:B:202:GLN:HB3	1:B:204:ARG:NH1	2.24	0.53
1:A:26:GLN:O	1:A:26:GLN:CD	2.51	0.53
1:A:173:TRP:O	1:A:177:LEU:HG	2.08	0.53
1:B:26:GLN:H	1:B:26:GLN:NE2	2.06	0.53
1:B:191:LEU:O	1:B:195:GLU:HG3	2.09	0.53
1:B:104:PHE:HD1	1:B:153:PHE:CZ	2.27	0.52
1:B:26:GLN:CD	1:B:26:GLN:N	2.68	0.52
1:B:145:ASN:HA	1:B:148:HIS:HD2	1.73	0.52
1:A:105:ASN:C	1:A:107:ILE:H	2.18	0.52
1:B:61:LEU:O	1:B:65:ILE:HG13	2.09	0.52
1:B:169:LEU:O	1:B:169:LEU:HD13	2.10	0.51
1:B:127:PRO:CG	1:B:175:VAL:CG1	2.51	0.51
1:A:32:GLN:CD	1:B:66:ARG:HH21	2.19	0.51
1:A:78:VAL:O	1:A:82:ARG:HD3	2.11	0.51
1:A:175:VAL:HG13	1:B:27:LEU:HB3	1.92	0.51
1:B:180:LEU:CD2	1:B:189:LEU:HD11	2.40	0.51
1:A:195:GLU:HA	1:A:209:LEU:HD11	1.93	0.51
1:B:188:LEU:N	1:B:188:LEU:HD12	2.25	0.51
1:A:32:GLN:HB2	1:B:66:ARG:NH2	2.26	0.51
1:A:49:THR:O	1:A:52:LEU:HB2	2.11	0.51
1:A:210:ASN:ND2	2:A:229:HOH:O	2.43	0.51
1:A:105:ASN:C	1:A:107:ILE:N	2.69	0.50
1:B:51:LEU:HD13	1:B:51:LEU:O	2.12	0.50
1:B:132:CYS:HB3	1:B:135:LYS:HB2	1.93	0.50
1:A:63:ARG:CG	1:A:64:ASP:N	2.74	0.50
1:A:79:GLU:O	1:A:83:LYS:HG3	2.11	0.50
1:A:92:PHE:HA	1:A:107:ILE:HD11	1.93	0.50
1:A:188:LEU:HD12	1:A:188:LEU:N	2.27	0.50
1:A:191:LEU:HG	1:A:212:LEU:HD12	1.94	0.50
1:A:81:LEU:CD2	1:A:118:LEU:HD22	2.41	0.50
1:B:35:LEU:HD13	1:B:35:LEU:O	2.12	0.50
1:A:202:GLN:HB2	1:A:204:ARG:NH1	2.27	0.49
1:B:171:GLY:O	1:B:175:VAL:HG23	2.12	0.49
1:B:127:PRO:CB	1:B:128:PRO:HD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:H	1:A:33:LEU:HD23	1.77	0.49
1:A:156:PRO:HA	1:A:159:ASN:HD22	1.78	0.49
1:B:131:THR:HG22	1:B:131:THR:O	2.13	0.49
1:A:135:LYS:O	1:A:138:THR:HB	2.12	0.49
1:A:160:VAL:HG23	1:A:161:TYR:N	2.27	0.48
1:A:195:GLU:OE1	1:A:209:LEU:HD11	2.12	0.48
1:A:190:PRO:HB3	1:A:193:GLU:HG3	1.94	0.48
1:A:175:VAL:CG1	1:B:27:LEU:HB3	2.43	0.48
1:B:107:ILE:HG22	1:B:107:ILE:O	2.13	0.48
1:B:191:LEU:HD12	1:B:216:GLN:OE1	2.14	0.48
1:A:178:ARG:O	1:A:181:GLU:HB2	2.13	0.47
1:B:51:LEU:HD13	1:B:51:LEU:C	2.40	0.47
1:A:135:LYS:HE3	1:A:135:LYS:HA	1.96	0.46
1:B:134:GLU:OE2	1:B:134:GLU:HA	2.15	0.46
1:B:122:VAL:HA	1:B:139:PHE:HE2	1.80	0.46
1:A:145:ASN:HD21	1:A:197:HIS:CE1	2.31	0.46
1:B:85:LEU:HD12	1:B:85:LEU:C	2.41	0.45
1:A:105:ASN:O	1:A:107:ILE:N	2.49	0.45
1:B:101:ASP:O	1:B:104:PHE:HB3	2.16	0.45
1:B:194:LEU:HA	1:B:197:HIS:HB2	1.98	0.45
1:A:127:PRO:O	1:A:128:PRO:CB	2.65	0.45
1:B:169:LEU:HD22	1:B:169:LEU:HA	1.69	0.45
1:B:81:LEU:HG	1:B:121:MSE:HE1	1.98	0.45
1:B:165:ALA:O	1:B:169:LEU:HB2	2.17	0.45
1:A:196:GLU:O	1:A:199:LYS:HG3	2.17	0.45
1:A:127:PRO:O	1:A:128:PRO:HB2	2.17	0.45
1:A:188:LEU:HD12	1:A:188:LEU:H	1.81	0.45
1:B:186:VAL:HA	1:B:187:PRO:HD3	1.84	0.45
1:A:169:LEU:O	1:A:173:TRP:HD1	2.00	0.44
1:B:188:LEU:N	1:B:188:LEU:CD1	2.81	0.44
1:A:43:ASP:OD2	1:A:45:GLN:HB2	2.17	0.44
1:A:117:ALA:CB	1:A:121:MSE:HE3	2.38	0.44
1:A:125:TYR:O	1:A:136:ASN:CG	2.61	0.44
1:B:131:THR:O	1:B:131:THR:CG2	2.66	0.44
1:A:33:LEU:HD23	1:A:33:LEU:N	2.33	0.44
1:A:61:LEU:O	1:A:65:ILE:HG13	2.18	0.44
1:A:132:CYS:SG	1:A:134:GLU:HG2	2.57	0.44
1:B:122:VAL:HA	1:B:139:PHE:CE2	2.53	0.44
1:B:125:TYR:HB3	1:B:136:ASN:HA	2.00	0.44
1:B:191:LEU:CD2	1:B:195:GLU:HG3	2.48	0.44
1:B:106:ARG:C	1:B:107:ILE:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:CG	1:B:204:ARG:NH1	2.75	0.43
1:A:179:GLN:HE21	1:A:179:GLN:HB2	1.63	0.43
1:B:45:GLN:O	1:B:48:PHE:HB3	2.18	0.43
1:B:211:TYR:HA	1:B:214:GLN:CD	2.43	0.43
1:B:189:LEU:HA	1:B:190:PRO:HD3	1.73	0.43
1:B:85:LEU:HD12	1:B:86:ILE:N	2.34	0.43
1:B:88:LEU:HD12	1:B:111:TYR:HA	2.01	0.43
1:A:136:ASN:O	1:A:137:ILE:C	2.62	0.43
1:A:167:TYR:O	1:A:170:THR:HB	2.18	0.43
1:A:180:LEU:CD2	1:A:189:LEU:HD11	2.49	0.43
1:A:93:PRO:O	1:A:94:TYR:C	2.62	0.42
1:B:31:GLU:CG	1:B:32:GLN:N	2.82	0.42
1:B:125:TYR:O	1:B:136:ASN:HB3	2.19	0.42
1:A:32:GLN:O	1:A:33:LEU:C	2.62	0.42
1:B:110:LYS:O	1:B:113:ALA:HB3	2.19	0.42
1:B:140:LEU:CD1	1:B:176:VAL:HG21	2.41	0.42
1:B:178:ARG:HG3	1:B:178:ARG:O	2.20	0.42
1:B:169:LEU:HD13	1:B:169:LEU:C	2.43	0.42
1:A:123:PRO:C	1:A:125:TYR:H	2.28	0.42
1:B:205:MSE:O	1:B:206:GLU:C	2.62	0.42
1:A:23:ARG:HG3	1:A:23:ARG:HH11	1.85	0.42
1:A:46:GLN:O	1:A:50:ILE:HG23	2.20	0.42
1:A:164:GLN:O	1:A:165:ALA:C	2.63	0.42
1:A:178:ARG:C	1:A:180:LEU:H	2.28	0.41
1:A:38:LEU:HD13	1:A:38:LEU:O	2.19	0.41
1:B:50:ILE:O	1:B:54:CYS:SG	2.70	0.41
1:B:88:LEU:HG	1:B:107:ILE:CG2	2.51	0.41
1:A:127:PRO:O	1:A:128:PRO:CG	2.68	0.41
1:A:45:GLN:C	1:A:45:GLN:NE2	2.73	0.41
1:B:133:PHE:CZ	1:B:137:ILE:HD11	2.56	0.41
1:A:27:LEU:HD23	1:B:175:VAL:CG2	2.46	0.41
1:A:51:LEU:C	1:A:51:LEU:CD2	2.94	0.40
1:B:33:LEU:HD12	1:B:33:LEU:HA	1.85	0.40
1:A:123:PRO:C	1:A:125:TYR:N	2.79	0.40
1:B:149:GLU:O	1:B:150:LEU:C	2.65	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ALA:O	1:A:157:ASN:ND2[1_666]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLN:NE2	1:B:18:GLU:O[1_455]	2.04	0.16

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	196/245 (80%)	166 (85%)	23 (12%)	7 (4%)	2	4
1	B	197/245 (80%)	169 (86%)	20 (10%)	8 (4%)	2	3
All	All	393/490 (80%)	335 (85%)	43 (11%)	15 (4%)	2	4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	128	PRO
1	A	185	VAL
1	B	19	ASP
1	B	94	TYR
1	B	127	PRO
1	B	185	VAL
1	B	25	ARG
1	B	214	GLN
1	A	66	ARG
1	B	93	PRO
1	A	67	GLY
1	A	187	PRO
1	B	45	GLN
1	A	59	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	178/218 (82%)	151 (85%)	27 (15%)	3	4
1	B	180/218 (83%)	154 (86%)	26 (14%)	3	5
All	All	358/436 (82%)	305 (85%)	53 (15%)	3	5

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	23	ARG
1	A	26	GLN
1	A	32	GLN
1	A	35	LEU
1	A	38	LEU
1	A	44	LYS
1	A	45	GLN
1	A	52	LEU
1	A	59	PRO
1	A	79	GLU
1	A	82	ARG
1	A	88	LEU
1	A	106	ARG
1	A	110	LYS
1	A	127	PRO
1	A	128	PRO
1	A	135	LYS
1	A	179	GLN
1	A	183	ARG
1	A	192	GLU
1	A	195	GLU
1	A	204	ARG
1	A	209	LEU
1	A	212	LEU
1	A	215	LEU
1	A	216	GLN

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Mol	Chain	Res	Type
1	B	23	ARG
1	B	26	GLN
1	B	29	VAL
1	B	35	LEU
1	B	39	LEU
1	B	52	LEU
1	B	75	ASP
1	B	79	GLU
1	B	80	THR
1	B	101	ASP
1	B	107	ILE
1	B	115	LEU
1	B	118	LEU
1	B	127	PRO
1	B	132	CYS
1	B	137	ILE
1	B	169	LEU
1	B	180	LEU
1	B	189	LEU
1	B	191	LEU
1	B	194	LEU
1	B	204	ARG
1	B	205	MSE
1	B	209	LEU
1	B	215	LEU
1	B	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	58	HIS
1	A	145	ASN
1	A	154	HIS
1	A	179	GLN
1	A	210	ASN
1	B	45	GLN
1	B	46	GLN
1	B	105	ASN
1	B	116	HIS
1	B	157	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 [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	194/245 (79%)	0.37	5 (2%) 57 55	31, 69, 105, 123	0
1	B	195/245 (79%)	0.28	3 (1%) 72 71	34, 68, 94, 106	0
All	All	389/490 (79%)	0.33	8 (2%) 63 61	31, 68, 99, 123	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	VAL	3.3
1	B	127	PRO	3.0
1	A	127	PRO	2.5
1	A	216	GLN	2.4
1	A	215	LEU	2.3
1	A	184	PRO	2.2
1	B	20	ILE	2.2
1	B	40	GLN	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.