WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 29, 2024 – 06:16 AM EDT

PDB ID	:	3RIU
Title	:	Crystal structure of Drosophila hexameric C3PO formed by truncated Translin and Trax
Authors	:	Tian, Y.; Simanshu, D.K.; Patel, D.J.
Deposited on	:	2011-04-14
Resolution	:	3.40 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.40 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	Percentile Ranks	Value
Rfree		0.338
Clashscore		32
Ramachandran outliers		2.4%
Sidechain outliers		9.1%
RSRZ outliers		11.9%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
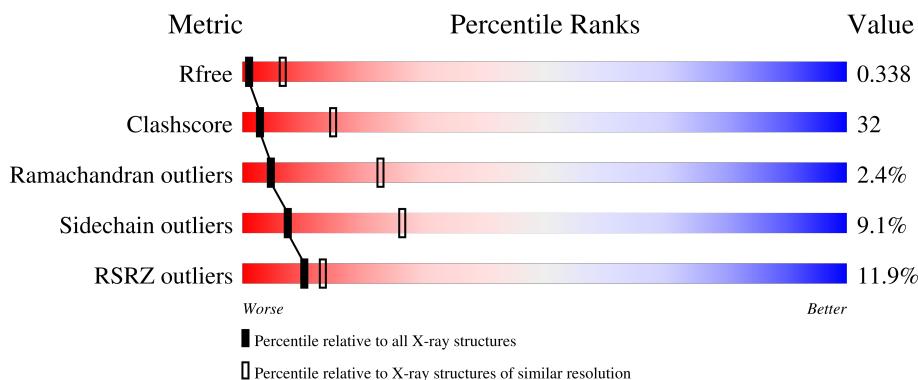
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_free	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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 <=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	218	9% / 58% / 34% / • 6%
1	B	218	10% / 46% / 42% / 6% / 7%
2	C	269	10% / 25% / 38% / 9% / 29%
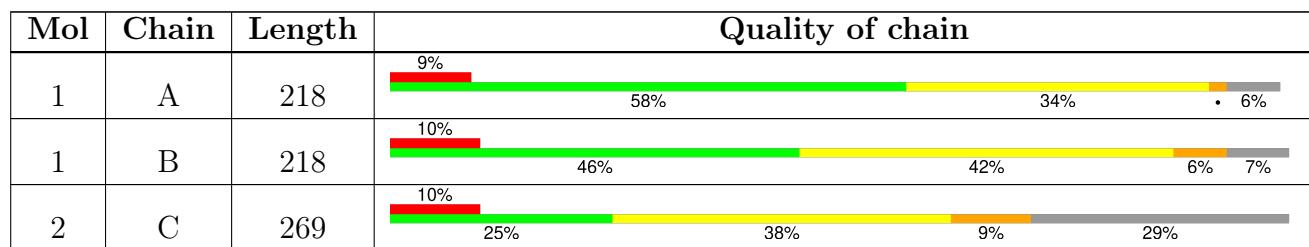
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4722 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 Translin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	Se	0	0	0
			1610	1030	270	306	2	2			
1	B	203	Total	C	N	O	S	Se	0	0	0
			1611	1032	268	307	2	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q7JVK6
B	0	SER	-	expression tag	UNP Q7JVK6

- Molecule 2 is a protein called Translin associated factor X, isoform B.

| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	190	Total	C	N	O	S	Se	0	0	0
			1501	955	265	270	6	5			

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: Translin
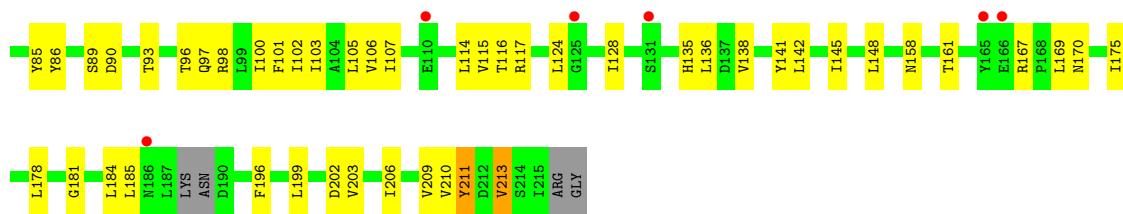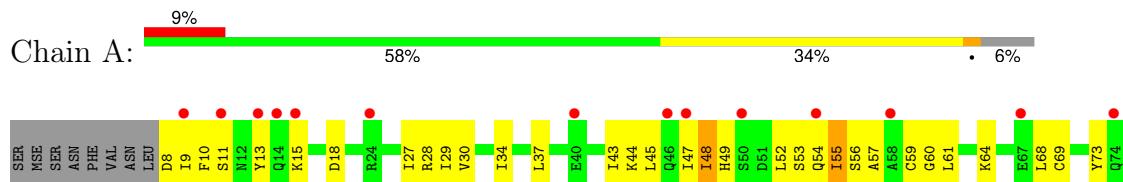
- Molecule 1: Translin
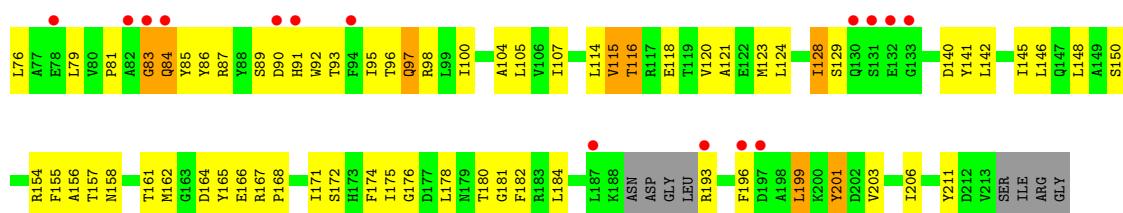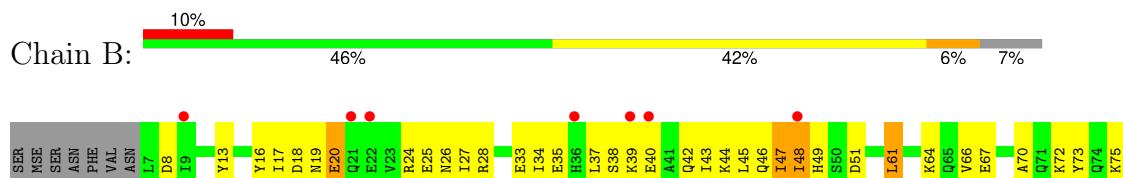
- Molecule 2: Translin associated factor X, isoform B
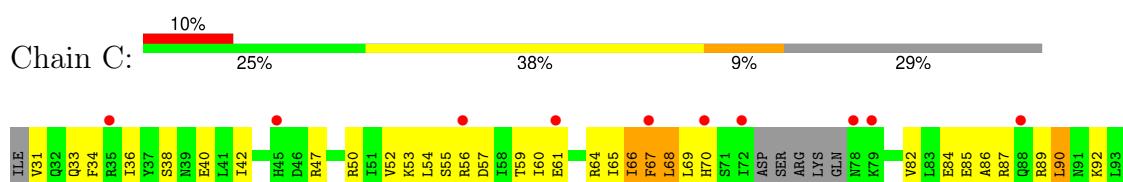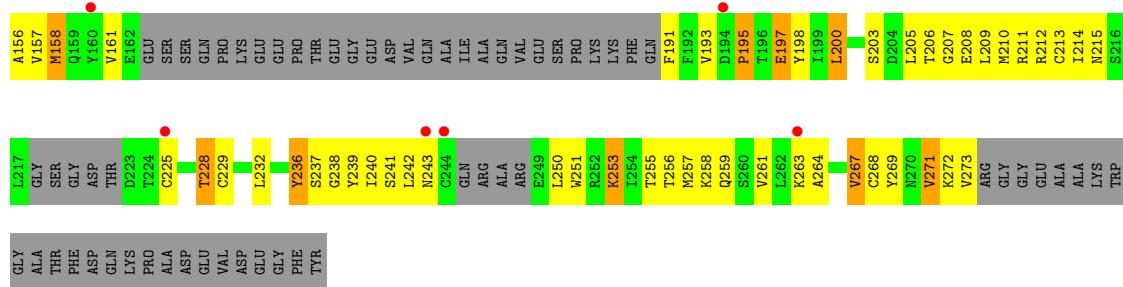
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	196.03Å 196.03Å 155.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 3.40 19.88 – 3.40	Depositor EDS
% Data completeness (in resolution range)	79.7 (19.88-3.40) 78.5 (19.88-3.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.271 , 0.338 0.268 , 0.338	Depositor DCC
R_{free} test set	1000 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 55.0	EDS
L-test for twinning[2]	$< |L| > = 0.35, < L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	4722	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

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	0.25	0/1634	0.41	0/2212
1	B	0.35	0/1636	0.53	0/2213
2	C	0.29	0/1512	0.46	0/2022
All	All	0.30	0/4782	0.47	0/6447

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

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	1610	0	1551	68	0
1	B	1611	0	1555	94	0
2	C	1501	0	1497	147	0
All	All	4722	0	4603	296	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 32.

All (296) 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)
2:C:114:ARG:HG2	2:C:117:TYR:CE2	1.60	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:SER:CB	2:C:119:PRO:CD	2.30	1.10
2:C:147:SER:HA	2:C:148:VAL:HG23	1.37	1.04
2:C:118:SER:CB	2:C:119:PRO:HD2	1.91	1.00
2:C:114:ARG:CG	2:C:117:TYR:CE2	2.45	0.99
1:B:51:ASP:HA	1:B:162:MSE:HE1	1.48	0.92
2:C:114:ARG:HG2	2:C:117:TYR:HE2	1.08	0.90
2:C:98:PHE:HD1	2:C:161:VAL:HG13	1.36	0.89
1:B:92:TRP:O	1:B:96:THR:HG23	1.72	0.88
1:A:45:LEU:HD13	1:A:105:LEU:HD23	1.55	0.87
1:B:27:ILE:HG23	1:B:76:LEU:HD11	1.56	0.86
2:C:195:PRO:HD2	2:C:197:GLU:HG2	1.59	0.83
1:B:73:TYR:OH	1:B:96:THR:HG22	1.76	0.83
1:B:49:HIS:CE1	1:B:154:ARG:HG2	2.13	0.82
1:A:100:ILE:HD13	1:A:141:TYR:HA	1.61	0.81
2:C:131:MSE:O	2:C:135:CYS:HB2	1.79	0.80
2:C:50:ARG:HD2	2:C:103:LEU:HD13	1.64	0.80
1:B:44:LYS:O	1:B:47:ILE:HG22	1.82	0.79
1:B:45:LEU:HA	1:B:48:ILE:HG23	1.65	0.78
2:C:146:LYS:HB2	2:C:148:VAL:HA	1.66	0.76
2:C:118:SER:CB	2:C:119:PRO:HD3	2.14	0.76
1:B:100:ILE:HD13	1:B:141:TYR:HA	1.68	0.75
2:C:98:PHE:CD1	2:C:161:VAL:HG13	2.23	0.74
1:A:117:ARG:HD2	1:A:128:ILE:HG23	1.68	0.73
1:B:193:ARG:HA	1:B:196:PHE:CE2	2.23	0.73
2:C:52:VAL:O	2:C:56:ARG:HG3	1.89	0.73
1:A:141:TYR:HD2	1:A:142:LEU:HD23	1.53	0.73
1:B:114:LEU:HD23	1:B:114:LEU:H	1.54	0.73
1:A:107:ILE:HD13	1:A:114:LEU:HA	1.71	0.71
2:C:111:TYR:HA	2:C:114:ARG:HG3	1.73	0.70
2:C:116:SER:C	2:C:118:SER:H	1.95	0.70
2:C:33:GLN:O	2:C:36:ILE:HG22	1.90	0.70
2:C:114:ARG:CG	2:C:117:TYR:HE2	1.94	0.69
1:B:49:HIS:CE1	1:B:155:PHE:HA	2.28	0.68
2:C:97:ASN:O	2:C:101:VAL:HG12	1.94	0.68
2:C:84:GLU:O	2:C:87:ARG:HG2	1.94	0.68
2:C:239:TYR:CD1	2:C:257:MSE:HE1	2.28	0.68
2:C:203:SER:HA	2:C:206:THR:HG23	1.77	0.67
1:B:193:ARG:HA	1:B:196:PHE:HE2	1.60	0.67
1:B:45:LEU:O	1:B:48:ILE:HG12	1.93	0.67
1:B:45:LEU:HD23	1:B:105:LEU:HD12	1.75	0.66
1:A:37:LEU:HD21	1:A:68:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TYR:CD2	1:A:142:LEU:HD23	2.30	0.66
1:B:35:GLU:HG2	1:B:39:LYS:HE3	1.77	0.65
1:B:42:GLN:NE2	2:C:240:ILE:HD11	2.10	0.65
2:C:147:SER:CA	2:C:148:VAL:HG23	2.20	0.65
1:B:13:TYR:O	1:B:17:ILE:HG23	1.96	0.65
2:C:116:SER:O	2:C:118:SER:N	2.30	0.65
2:C:66:ILE:HG22	2:C:127:ALA:HB2	1.79	0.64
2:C:89:ARG:O	2:C:92:LYS:HG2	1.97	0.64
2:C:114:ARG:HB3	2:C:117:TYR:CD2	2.32	0.64
2:C:129:THR:CG2	2:C:205:LEU:HG	2.27	0.64
1:B:34:ILE:HD11	1:B:72:LYS:HB3	1.79	0.64
2:C:118:SER:O	2:C:120:GLY:N	2.30	0.64
1:A:116:THR:HA	1:A:141:TYR:OH	1.98	0.64
1:A:98:ARG:O	1:A:102:ILE:HG12	1.98	0.64
1:B:174:PHE:CD2	1:B:175:ILE:HD12	2.33	0.63
1:B:199:LEU:C	1:B:199:LEU:HD12	2.20	0.63
1:B:49:HIS:HE1	1:B:155:PHE:HA	1.63	0.63
2:C:67:PHE:HA	2:C:70:HIS:HD2	1.64	0.62
1:A:10:PHE:HA	1:A:13:TYR:CD2	2.34	0.62
2:C:65:ILE:CD1	2:C:90:LEU:HD12	2.30	0.62
2:C:114:ARG:CB	2:C:117:TYR:CD2	2.82	0.62
1:A:184:LEU:HD21	2:C:34:PHE:HB2	1.81	0.62
2:C:158:MSE:HA	2:C:158:MSE:HE2	1.80	0.62
2:C:60:ILE:O	2:C:64:ARG:HG3	2.00	0.62
2:C:129:THR:HG22	2:C:205:LEU:HG	1.82	0.61
1:B:199:LEU:O	1:B:203:VAL:HG23	1.99	0.61
1:B:96:THR:O	1:B:100:ILE:HG13	2.00	0.61
2:C:57:ASP:O	2:C:61:GLU:HB2	1.99	0.61
2:C:94:ILE:HG23	2:C:158:MSE:CE	2.30	0.61
2:C:130:TYR:CZ	2:C:134:LEU:HD23	2.34	0.61
1:A:44:LYS:O	1:A:47:ILE:HB	2.01	0.60
1:A:184:LEU:HD11	2:C:34:PHE:HB3	1.83	0.60
1:B:174:PHE:HD2	1:B:175:ILE:HD12	1.64	0.60
2:C:111:TYR:HA	2:C:114:ARG:CG	2.31	0.60
1:B:17:ILE:HG13	1:B:18:ASP:N	2.16	0.60
2:C:65:ILE:HD12	2:C:90:LEU:HD12	1.83	0.60
1:A:8:ASP:OD1	2:C:146:LYS:HA	2.01	0.60
1:B:49:HIS:CD2	1:B:154:ARG:HE	2.18	0.60
1:B:66:VAL:HG11	1:B:123:MSE:HE2	1.83	0.60
2:C:90:LEU:HD21	2:C:128:TYR:HA	1.84	0.60
2:C:101:VAL:HG21	2:C:191:PHE:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:O	1:B:46:GLN:HB2	2.02	0.59
1:A:181:GLY:O	2:C:34:PHE:HD1	1.84	0.59
1:A:211:TYR:HD1	1:A:211:TYR:O	1.84	0.59
1:A:103:ILE:O	1:A:107:ILE:HG13	2.03	0.59
2:C:259:GLN:O	2:C:263:LYS:HG3	2.03	0.58
2:C:68:LEU:HD23	2:C:69:LEU:N	2.19	0.58
1:B:83:GLY:O	1:B:85:TYR:N	2.36	0.58
2:C:130:TYR:OH	2:C:212:ARG:HB2	2.04	0.58
1:B:20:GLU:OE2	1:B:87:ARG:HD2	2.05	0.57
1:B:39:LYS:O	1:B:43:ILE:HG23	2.04	0.57
1:A:49:HIS:HB3	1:A:158:ASN:ND2	2.20	0.57
1:A:60:GLY:O	1:A:64:LYS:HB2	2.05	0.57
2:C:111:TYR:HD1	2:C:114:ARG:HD2	1.70	0.57
1:A:211:TYR:HD1	1:A:211:TYR:C	2.08	0.56
1:A:206:ILE:O	1:A:210:VAL:HG23	2.06	0.56
1:B:39:LYS:NZ	2:C:243:ASN:HA	2.20	0.56
2:C:213:CYS:HB2	2:C:228:THR:HG21	1.87	0.56
2:C:31:VAL:HG23	2:C:33:GLN:H	1.70	0.56
2:C:263:LYS:O	2:C:267:VAL:HG13	2.05	0.56
2:C:114:ARG:CB	2:C:117:TYR:CE2	2.88	0.56
1:A:57:ALA:O	1:A:61:LEU:HD13	2.05	0.56
1:B:171:ILE:HG22	1:B:206:ILE:HD13	1.87	0.56
1:B:25:GLU:HA	1:B:28:ARG:HD2	1.86	0.56
1:B:142:LEU:HD22	1:B:182:PHE:CE1	2.41	0.55
2:C:119:PRO:O	2:C:123:GLU:N	2.33	0.55
1:A:100:ILE:HD11	1:A:136:LEU:HD11	1.87	0.55
1:B:39:LYS:HZ1	2:C:243:ASN:HA	1.70	0.55
1:A:185:LEU:HD23	2:C:38:SER:HB2	1.88	0.55
2:C:118:SER:O	2:C:119:PRO:C	2.45	0.55
2:C:130:TYR:HA	2:C:205:LEU:HD21	1.87	0.55
1:B:45:LEU:CD2	1:B:105:LEU:HD12	2.36	0.55
2:C:38:SER:O	2:C:42:ILE:HG13	2.06	0.55
1:A:181:GLY:O	1:A:184:LEU:HG	2.07	0.55
2:C:232:LEU:HB3	2:C:261:VAL:HG22	1.88	0.55
2:C:104:GLU:C	2:C:105:LEU:HD12	2.28	0.55
2:C:207:GLY:O	2:C:211:ARG:HG3	2.07	0.55
2:C:237:SER:O	2:C:241:SER:HB3	2.07	0.55
1:B:73:TYR:CZ	1:B:96:THR:HG22	2.41	0.54
1:B:81:PRO:HG2	1:B:84:GLN:HG3	1.88	0.54
1:A:27:ILE:HD12	1:A:28:ARG:N	2.23	0.54
2:C:84:GLU:HA	2:C:87:ARG:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HD13	1:A:73:TYR:CE1	2.43	0.54
1:A:103:ILE:HG22	1:A:115:VAL:HG21	1.89	0.54
1:B:114:LEU:H	1:B:114:LEU:CD2	2.19	0.54
1:B:40:GLU:O	1:B:43:ILE:HG12	2.07	0.54
1:B:104:ALA:HA	1:B:115:VAL:HG22	1.90	0.54
2:C:116:SER:C	2:C:118:SER:N	2.60	0.54
1:A:211:TYR:C	1:A:211:TYR:CD1	2.79	0.54
2:C:111:TYR:CD1	2:C:114:ARG:HD2	2.43	0.53
2:C:36:ILE:O	2:C:40:GLU:HB2	2.09	0.53
2:C:119:PRO:O	2:C:123:GLU:HB2	2.09	0.53
1:A:59:CYS:SG	1:A:106:VAL:HG13	2.49	0.53
1:B:145:ILE:O	1:B:148:LEU:HB3	2.09	0.53
1:B:34:ILE:HD11	1:B:72:LYS:CB	2.38	0.53
1:B:61:LEU:O	1:B:64:LYS:HG2	2.09	0.53
1:B:97:GLN:NE2	1:B:140:ASP:HA	2.23	0.53
2:C:130:TYR:O	2:C:134:LEU:HG	2.08	0.53
1:B:142:LEU:HD23	1:B:145:ILE:HD11	1.91	0.52
2:C:211:ARG:O	2:C:214:ILE:HG22	2.08	0.52
1:A:175:ILE:HG23	1:A:203:VAL:HG22	1.92	0.52
2:C:47:ARG:HH22	2:C:105:LEU:HD13	1.74	0.52
2:C:212:ARG:O	2:C:215:ASN:HB2	2.10	0.52
1:A:107:ILE:CD1	1:A:114:LEU:HA	2.37	0.52
2:C:50:ARG:O	2:C:53:LYS:HB2	2.09	0.52
1:B:128:ILE:HD13	1:B:128:ILE:C	2.30	0.52
1:A:184:LEU:HD12	1:A:184:LEU:C	2.30	0.52
1:B:83:GLY:C	1:B:85:TYR:H	2.12	0.52
2:C:95:ALA:O	2:C:98:PHE:HB3	2.10	0.52
1:A:145:ILE:O	1:A:148:LEU:HB3	2.11	0.51
2:C:114:ARG:O	2:C:117:TYR:HB2	2.10	0.51
1:A:10:PHE:CD1	1:A:13:TYR:HD2	2.29	0.51
1:B:95:ILE:O	1:B:98:ARG:HB3	2.10	0.51
1:B:34:ILE:HG21	1:B:73:TYR:HE1	1.75	0.51
1:B:35:GLU:HB2	1:B:95:ILE:HD11	1.92	0.51
1:B:100:ILE:HD13	1:B:141:TYR:CA	2.40	0.51
1:A:114:LEU:HD13	1:A:178:LEU:HD21	1.93	0.51
1:B:73:TYR:OH	1:B:96:THR:CG2	2.54	0.51
1:B:33:GLU:O	1:B:37:LEU:HD13	2.11	0.51
2:C:103:LEU:HD23	2:C:103:LEU:H	1.76	0.51
1:B:193:ARG:HA	1:B:196:PHE:CD2	2.46	0.50
2:C:131:MSE:O	2:C:135:CYS:CB	2.56	0.50
1:B:86:TYR:HA	1:B:89:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:VAL:O	2:C:104:GLU:HB2	2.11	0.50
2:C:117:TYR:O	2:C:118:SER:O	2.30	0.50
2:C:31:VAL:HG23	2:C:33:GLN:HB2	1.93	0.50
1:B:172:SER:HB2	1:B:206:ILE:HG22	1.94	0.50
2:C:151:TRP:HB3	2:C:198:TYR:CB	2.42	0.50
2:C:271:VAL:O	2:C:273:VAL:N	2.45	0.49
1:B:107:ILE:HG12	1:B:115:VAL:CG1	2.42	0.49
2:C:82:VAL:O	2:C:86:ALA:CB	2.60	0.49
1:A:48:ILE:HG13	1:A:48:ILE:O	2.12	0.49
1:A:199:LEU:O	1:A:203:VAL:HG23	2.12	0.49
1:B:167:ARG:HB2	1:B:168:PRO:HD3	1.94	0.49
1:A:101:PHE:HE1	1:A:148:LEU:HA	1.78	0.49
2:C:55:SER:O	2:C:59:THR:HG22	2.12	0.49
1:B:8:ASP:OD1	1:B:8:ASP:N	2.45	0.49
2:C:128:TYR:O	2:C:131:MSE:HB3	2.13	0.49
2:C:114:ARG:HA	2:C:117:TYR:CD2	2.49	0.48
1:A:107:ILE:HG12	1:A:115:VAL:HG13	1.95	0.48
1:A:85:TYR:O	1:A:89:SER:HB3	2.13	0.48
1:B:89:SER:O	1:B:93:THR:HG23	2.13	0.48
2:C:94:ILE:HG23	2:C:158:MSE:HE1	1.95	0.48
2:C:34:PHE:N	2:C:34:PHE:CD2	2.81	0.48
2:C:52:VAL:HG12	2:C:56:ARG:HE	1.77	0.48
1:B:156:ALA:HB2	1:B:171:ILE:HD12	1.95	0.48
1:A:209:VAL:O	1:A:213:VAL:HG23	2.14	0.48
1:B:92:TRP:O	1:B:96:THR:CG2	2.54	0.48
1:B:105:LEU:HA	1:B:148:LEU:HD13	1.96	0.48
2:C:130:TYR:CE1	2:C:134:LEU:HD23	2.48	0.48
1:B:16:TYR:O	1:B:19:ASN:HB3	2.14	0.47
1:B:176:GLY:O	1:B:180:THR:HG23	2.14	0.47
1:A:29:ILE:HG13	1:A:30:VAL:N	2.30	0.47
1:A:10:PHE:CE2	2:C:238:GLY:HA3	2.50	0.47
2:C:34:PHE:N	2:C:34:PHE:HD2	2.12	0.47
2:C:111:TYR:HA	2:C:114:ARG:CD	2.44	0.47
1:B:73:TYR:CE2	1:B:96:THR:HG22	2.49	0.47
1:B:158:ASN:HA	1:B:161:THR:HB	1.97	0.47
1:A:138:VAL:O	1:A:141:TYR:HB3	2.15	0.47
2:C:54:LEU:HD13	2:C:100:ALA:CA	2.45	0.47
1:A:37:LEU:HD13	1:A:69:CYS:HA	1.97	0.46
1:A:86:TYR:O	2:C:111:TYR:HB3	2.15	0.46
1:B:107:ILE:HG12	1:B:115:VAL:HG13	1.97	0.46
2:C:134:LEU:HD12	2:C:135:CYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:ALA:O	2:C:156:ALA:HB3	2.14	0.46
1:A:11:SER:O	1:A:15:LYS:HB2	2.16	0.46
1:B:118:GLU:O	1:B:121:ALA:HB3	2.15	0.46
2:C:53:LYS:HD2	2:C:56:ARG:CZ	2.45	0.46
2:C:114:ARG:HA	2:C:117:TYR:CE2	2.49	0.46
2:C:207:GLY:O	2:C:210:MSE:HB3	2.16	0.46
1:B:72:LYS:O	1:B:75:LYS:HB3	2.16	0.46
2:C:200:LEU:HD13	2:C:250:LEU:HD22	1.97	0.46
1:A:52:LEU:C	1:A:54:GLN:H	2.19	0.46
1:A:93:THR:O	1:A:97:GLN:HG3	2.15	0.46
1:A:103:ILE:HD11	1:A:124:LEU:HD21	1.98	0.46
1:B:67:GLU:O	1:B:70:ALA:HB3	2.16	0.46
2:C:92:LYS:O	2:C:95:ALA:HB3	2.16	0.45
1:B:178:LEU:HD21	1:B:182:PHE:HE2	1.80	0.45
2:C:82:VAL:O	2:C:86:ALA:HB2	2.15	0.45
2:C:147:SER:N	2:C:148:VAL:HA	2.31	0.45
1:A:101:PHE:CE1	1:A:148:LEU:HA	2.50	0.45
2:C:158:MSE:HA	2:C:158:MSE:CE	2.47	0.45
1:B:165:TYR:N	1:B:165:TYR:CD2	2.84	0.45
1:A:107:ILE:HG12	1:A:115:VAL:HG22	1.98	0.44
1:B:161:THR:OG1	2:C:269:TYR:HB2	2.17	0.44
1:A:96:THR:O	1:A:100:ILE:HG13	2.16	0.44
2:C:65:ILE:HD11	2:C:89:ARG:HG2	1.99	0.44
2:C:253:LYS:O	2:C:256:THR:HG22	2.16	0.44
1:A:86:TYR:HB2	2:C:110:VAL:HG12	1.99	0.44
1:A:213:VAL:HG12	1:A:213:VAL:O	2.18	0.44
2:C:67:PHE:HA	2:C:67:PHE:HD1	1.66	0.44
1:A:107:ILE:C	1:A:107:ILE:HD12	2.38	0.44
1:B:201:TYR:CD2	1:B:201:TYR:C	2.91	0.44
2:C:267:VAL:CG2	2:C:268:CYS:N	2.80	0.44
1:A:10:PHE:CG	1:A:13:TYR:HD2	2.36	0.44
1:B:178:LEU:O	1:B:181:GLY:N	2.51	0.43
2:C:200:LEU:CD1	2:C:250:LEU:HD22	2.48	0.43
1:A:141:TYR:O	1:A:145:ILE:HG12	2.18	0.43
1:A:161:THR:HG22	1:A:161:THR:O	2.18	0.43
1:A:202:ASP:O	1:A:206:ILE:HG13	2.17	0.43
2:C:68:LEU:HD21	2:C:86:ALA:HB2	1.99	0.43
2:C:251:TRP:O	2:C:255:THR:HG23	2.17	0.43
1:B:49:HIS:HE1	1:B:155:PHE:CA	2.30	0.43
2:C:54:LEU:HD13	2:C:100:ALA:HA	2.00	0.43
2:C:128:TYR:CD1	2:C:128:TYR:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:LEU:HB2	2:C:232:LEU:HD11	2.00	0.43
2:C:133:TYR:CB	2:C:147:SER:HB3	2.49	0.43
1:B:107:ILE:HD12	1:B:107:ILE:N	2.34	0.43
2:C:50:ARG:HD2	2:C:103:LEU:CD1	2.42	0.43
2:C:56:ARG:O	2:C:59:THR:HG22	2.18	0.43
2:C:205:LEU:HD13	2:C:205:LEU:C	2.38	0.43
1:B:158:ASN:O	1:B:162:MSE:HG2	2.19	0.43
2:C:114:ARG:CA	2:C:117:TYR:CD2	3.02	0.43
2:C:205:LEU:HD13	2:C:205:LEU:O	2.19	0.43
2:C:213:CYS:SG	2:C:225:CYS:HB2	2.58	0.43
1:A:43:ILE:CG2	1:A:44:LYS:N	2.81	0.42
1:B:24:ARG:C	1:B:26:ASN:H	2.21	0.42
1:B:45:LEU:CD1	1:B:45:LEU:N	2.82	0.42
1:B:37:LEU:O	1:B:38:SER:C	2.58	0.42
2:C:65:ILE:HD13	2:C:90:LEU:HD12	2.01	0.42
2:C:203:SER:CA	2:C:206:THR:HG23	2.47	0.42
1:B:116:THR:O	1:B:120:VAL:HG23	2.19	0.42
2:C:96:VAL:O	2:C:99:ARG:HB2	2.19	0.42
2:C:146:LYS:H	2:C:146:LYS:HG3	1.57	0.42
2:C:134:LEU:CD1	2:C:134:LEU:C	2.87	0.42
2:C:236:TYR:OH	2:C:258:LYS:HD2	2.19	0.42
1:A:175:ILE:CG2	1:A:203:VAL:HG22	2.48	0.42
1:B:178:LEU:HD21	1:B:182:PHE:CE2	2.55	0.42
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.94	0.42
2:C:208:GLU:HA	2:C:211:ARG:CD	2.50	0.42
2:C:68:LEU:CD2	2:C:86:ALA:HB2	2.50	0.42
2:C:236:TYR:CE1	2:C:258:LYS:HG3	2.54	0.42
2:C:193:VAL:HG12	2:C:195:PRO:HD3	2.02	0.42
1:B:123:MSE:HE2	1:B:123:MSE:HB3	1.95	0.41
2:C:134:LEU:HD12	2:C:134:LEU:C	2.40	0.41
1:A:142:LEU:O	1:A:145:ILE:HB	2.20	0.41
1:B:70:ALA:HB2	1:B:124:LEU:HA	2.03	0.41
1:B:35:GLU:HB2	1:B:95:ILE:CD1	2.50	0.41
1:B:42:GLN:HE21	2:C:240:ILE:HD11	1.85	0.41
2:C:67:PHE:O	2:C:70:HIS:HB2	2.20	0.41
1:B:164:ASP:OD1	1:B:166:GLU:HB3	2.20	0.41
2:C:84:GLU:HA	2:C:87:ARG:HD3	2.03	0.41
1:B:128:ILE:HG23	1:B:129:SER:N	2.36	0.41
2:C:31:VAL:CG2	2:C:33:GLN:HB2	2.51	0.41
1:A:15:LYS:HA	1:A:18:ASP:HB2	2.02	0.41
1:A:55:ILE:O	1:A:56:SER:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:O	1:A:199:LEU:HB3	2.20	0.41
2:C:66:ILE:HG22	2:C:127:ALA:CB	2.49	0.41
2:C:65:ILE:HG21	2:C:90:LEU:HD13	2.02	0.40
1:A:169:LEU:O	1:A:170:ASN:C	2.60	0.40
2:C:149:SER:O	2:C:150:ASP:CB	2.68	0.40
2:C:264:ALA:O	2:C:267:VAL:HG22	2.21	0.40
2:C:154:ILE:O	2:C:157:VAL:HG22	2.22	0.40
1:B:104:ALA:HB1	1:B:148:LEU:HD22	2.02	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	202/218 (93%)	176 (87%)	21 (10%)	5 (2%)	4	22
1	B	199/218 (91%)	176 (88%)	21 (11%)	2 (1%)	13	39
2	C	176/269 (65%)	153 (87%)	16 (9%)	7 (4%)	2	15
All	All	577/705 (82%)	505 (88%)	58 (10%)	14 (2%)	5	23

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	117	TYR
2	C	118	SER
2	C	195	PRO
1	A	55	ILE
1	B	83	GLY
2	C	148	VAL
2	C	272	LYS
1	A	53	SER
1	B	84	GLN

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Mol	Chain	Res	Type
2	C	119	PRO
1	A	213	VAL
1	A	90	ASP
2	C	271	VAL
1	A	9	ILE

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	166/191 (87%)	162 (98%)	4 (2%)	44	66
1	B	168/191 (88%)	151 (90%)	17 (10%)	6	22
2	C	161/235 (68%)	137 (85%)	24 (15%)	2	9
All	All	495/617 (80%)	450 (91%)	45 (9%)	7	26

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	135	HIS
1	A	167	ARG
1	A	211	TYR
1	B	20	GLU
1	B	47	ILE
1	B	48	ILE
1	B	61	LEU
1	B	90	ASP
1	B	91	HIS
1	B	97	GLN
1	B	115	VAL
1	B	116	THR
1	B	128	ILE
1	B	146	LEU
1	B	150	SER
1	B	157	THR

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Mol	Chain	Res	Type
1	B	184	LEU
1	B	199	LEU
1	B	201	TYR
1	B	211	TYR
2	C	66	ILE
2	C	67	PHE
2	C	68	LEU
2	C	85	GLU
2	C	90	LEU
2	C	97	ASN
2	C	103	LEU
2	C	116	SER
2	C	121	LEU
2	C	122	GLN
2	C	128	TYR
2	C	134	LEU
2	C	136	HIS
2	C	146	LYS
2	C	152	GLN
2	C	158	MSE
2	C	197	GLU
2	C	200	LEU
2	C	228	THR
2	C	229	CYS
2	C	236	TYR
2	C	242	LEU
2	C	253	LYS
2	C	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	91	HIS
1	A	97	GLN
1	A	135	HIS
1	A	158	ASN
1	B	49	HIS
1	B	97	GLN
2	C	70	HIS
2	C	97	ASN
2	C	112	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	204/218 (93%)	0.49	20 (9%)	14	16	45, 96, 190, 239	0
1	B	201/218 (92%)	0.28	22 (10%)	12	14	27, 58, 146, 228	0
2	C	185/269 (68%)	0.81	28 (15%)	6	9	26, 95, 205, 313	0
All	All	590/705 (83%)	0.52	70 (11%)	10	13	26, 84, 188, 313	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	112	GLN	6.3
2	C	160	TYR	5.7
2	C	244	CYS	5.3
2	C	119	PRO	5.1
1	B	196	PHE	4.5
1	B	133	GLY	4.5
2	C	111	TYR	4.4
1	A	166	GLU	3.9
1	A	67	GLU	3.9
1	A	125	GLY	3.8
2	C	120	GLY	3.8
1	B	90	ASP	3.8
2	C	78	ASN	3.8
2	C	114	ARG	3.8
1	B	131	SER	3.7
1	A	24	ARG	3.7
2	C	194	ASP	3.7
1	A	54	GLN	3.7
2	C	61	GLU	3.6
2	C	243	ASN	3.6
1	A	14	GLN	3.5
2	C	70	HIS	3.5
1	A	11	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	165	TYR	3.2
1	A	15	LYS	3.2
2	C	145	THR	3.2
1	A	74	GLN	3.2
1	A	50	SER	3.1
1	B	132	GLU	3.1
1	A	131	SER	3.1
2	C	263	LYS	3.1
2	C	79	LYS	3.1
1	B	91	HIS	3.1
2	C	225	CYS	3.0
1	B	84	GLN	3.0
1	A	47	ILE	3.0
1	B	22	GLU	3.0
2	C	116	SER	3.0
2	C	99	ARG	3.0
1	B	82	ALA	2.9
2	C	72	ILE	2.9
1	A	58	ALA	2.8
2	C	45	HIS	2.8
1	A	13	TYR	2.7
2	C	105	LEU	2.7
2	C	88	GLN	2.7
2	C	35	ARG	2.7
1	B	40	GLU	2.6
2	C	95	ALA	2.6
1	B	21	GLN	2.6
2	C	67	PHE	2.5
1	A	40	GLU	2.5
2	C	113	PHE	2.4
1	B	83	GLY	2.4
2	C	56	ARG	2.4
1	B	36	HIS	2.3
1	B	78	GLU	2.2
2	C	147	SER	2.2
1	B	94	PHE	2.2
1	A	9	ILE	2.1
1	B	130	GLN	2.1
1	A	110	GLU	2.1
1	B	48	ILE	2.1
1	A	46	GLN	2.1
1	A	186	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	193	ARG	2.1
1	B	197	ASP	2.1
1	B	187	LEU	2.1
1	B	9	ILE	2.0
1	B	39	LYS	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.