



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 AM UTC

PDB ID : 3TT6 / pdb_00003tt6
Title : Structure of ClpP from Bacillus subtilis in compressed state
Authors : Lee, B.-G.; Kim, M.K.; Song, H.K.
Deposited on : 2011-09-14
Resolution : 2.59 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

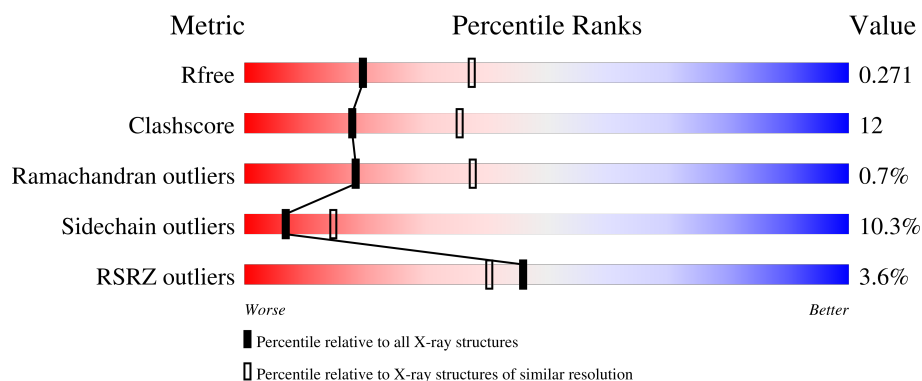
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
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	196	4% 60% 19% • 17%
1	B	196	5% 58% 21% • 17%
1	C	196	3% 61% 18% • 18%
1	D	196	2% 59% 19% 5% • 17%
1	E	196	4% 61% 17% • 18%

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Mol	Chain	Length	Quality of chain
1	F	196	3% 53% 22% 6% 18%
1	G	196	2% 55% 23% • • 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8602 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1228	780	205	236	7			
1	B	162	Total	C	N	O	S	0	0	0
			1228	780	205	236	7			
1	C	161	Total	C	N	O	S	0	0	0
			1223	777	204	235	7			
1	D	162	Total	C	N	O	S	0	0	0
			1233	783	207	236	7			
1	E	160	Total	C	N	O	S	0	0	0
			1216	772	203	234	7			
1	F	160	Total	C	N	O	S	0	0	0
			1218	774	203	234	7			
1	G	161	Total	C	N	O	S	0	0	0
			1228	780	206	235	7			

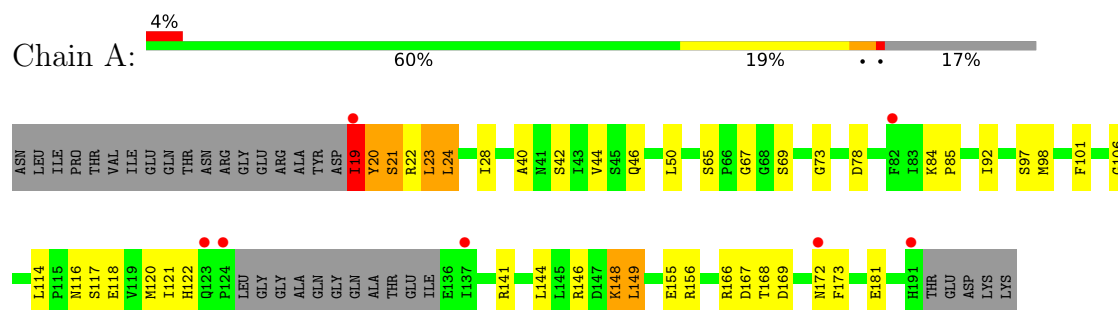
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	3	Total	O	0	0
			3	3		
2	C	6	Total	O	0	0
			6	6		
2	D	6	Total	O	0	0
			6	6		
2	E	3	Total	O	0	0
			3	3		
2	F	3	Total	O	0	0
			3	3		

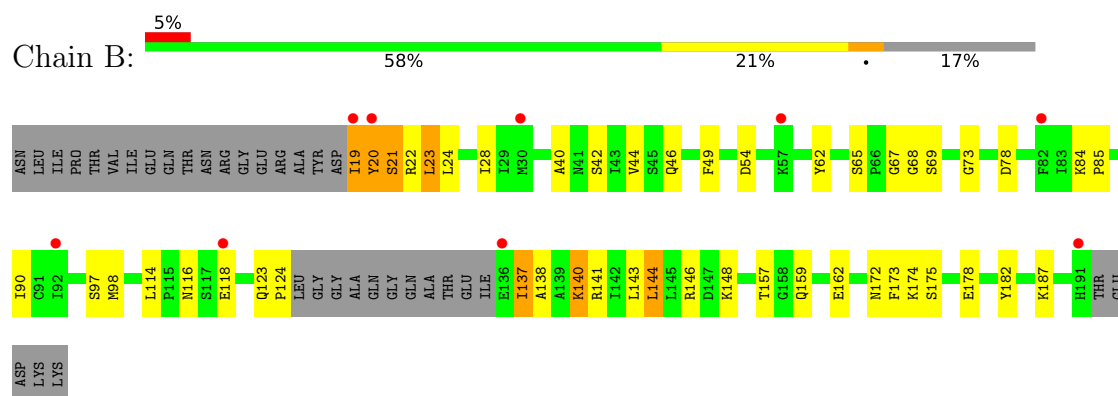
3 Residue-property plots [i](#)

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.

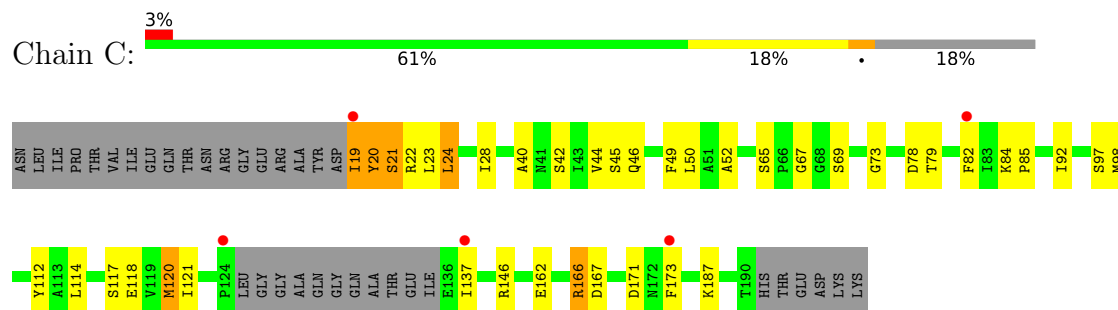
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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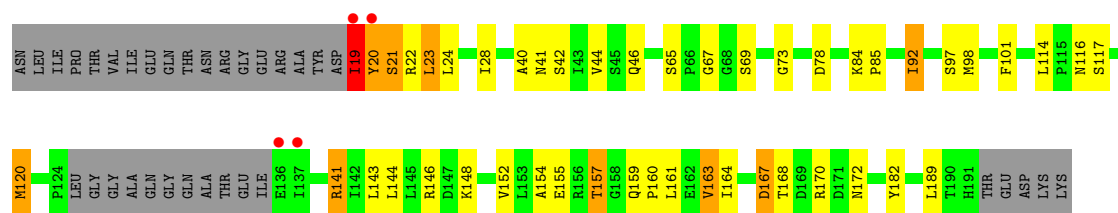


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

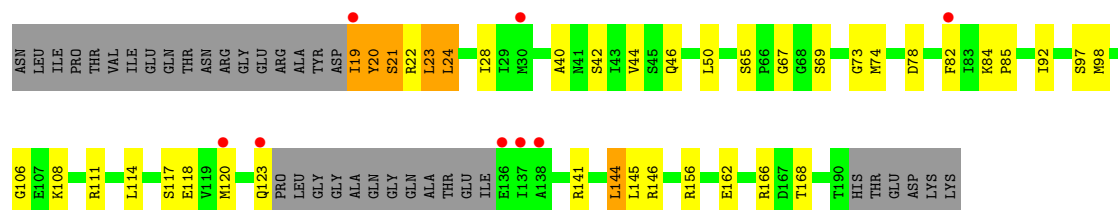


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

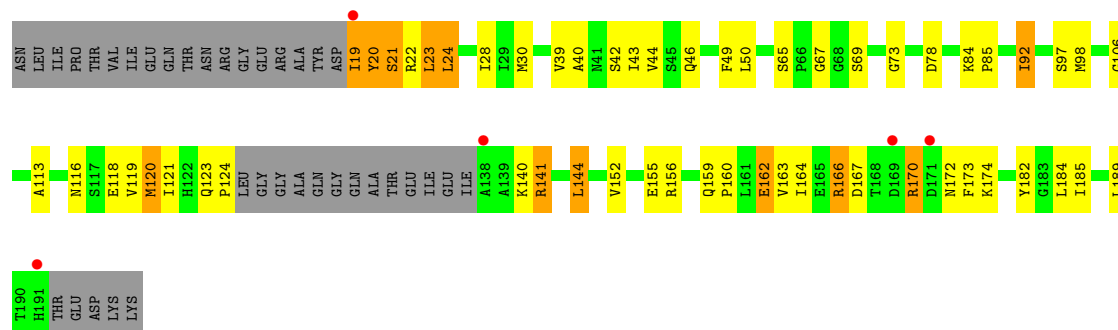




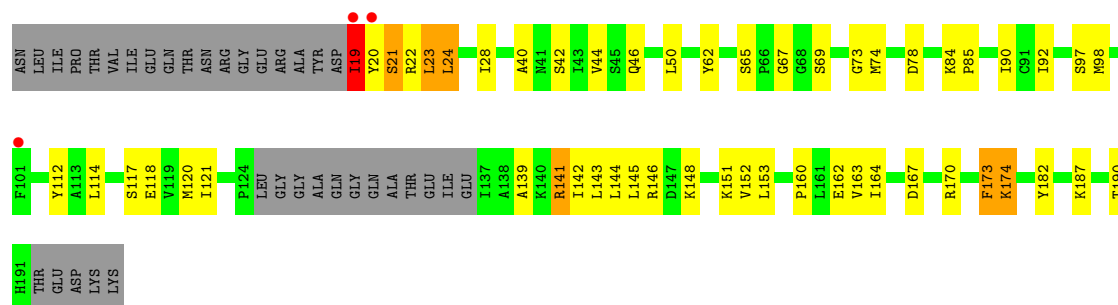
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.09Å 172.86Å 83.43Å 90.00° 118.93° 90.00°	Depositor
Resolution (Å)	36.09 – 2.59 36.09 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (36.09-2.59) 98.8 (36.09-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, R_{free}	0.221 , 0.277 0.215 , 0.271	Depositor DCC
R_{free} test set	2002 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k+l,3/2*h-1/2*k+l,-l 0.000 for 1/2*h-1/2*k+l,-3/2*h-1/2*k-l,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8602	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	0.82	0/1242	1.09	2/1675 (0.1%)
1	B	0.73	0/1242	1.06	6/1675 (0.4%)
1	C	0.83	0/1237	1.09	2/1668 (0.1%)
1	D	0.78	1/1248 (0.1%)	1.07	3/1683 (0.2%)
1	E	0.76	0/1229	1.06	2/1656 (0.1%)
1	F	0.75	1/1232 (0.1%)	1.01	2/1661 (0.1%)
1	G	0.69	0/1243	1.01	2/1676 (0.1%)
All	All	0.77	2/8673 (0.0%)	1.06	19/11694 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
1	G	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	41	ASN	CG-ND2	-6.43	1.19	1.33
1	F	92	ILE	CA-CB	-5.05	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	SER	CA-C-N	6.65	126.79	119.87
1	A	65	SER	C-N-CA	6.65	126.79	119.87
1	E	65	SER	CA-C-N	6.65	126.78	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	65	SER	C-N-CA	6.65	126.78	119.87
1	D	65	SER	CA-C-N	6.41	126.53	119.87
1	D	65	SER	C-N-CA	6.41	126.53	119.87
1	B	137	ILE	N-CA-C	6.26	116.63	107.75
1	G	65	SER	CA-C-N	6.14	126.26	119.87
1	G	65	SER	C-N-CA	6.14	126.26	119.87
1	F	65	SER	CA-C-N	5.95	126.05	119.87
1	F	65	SER	C-N-CA	5.95	126.05	119.87
1	B	68	GLY	N-CA-C	5.54	117.38	110.29
1	B	65	SER	CA-C-N	5.48	125.57	119.87
1	B	65	SER	C-N-CA	5.48	125.57	119.87
1	C	65	SER	CA-C-N	5.35	125.44	119.87
1	C	65	SER	C-N-CA	5.35	125.44	119.87
1	B	54	ASP	CA-C-N	5.28	125.08	119.28
1	B	54	ASP	C-N-CA	5.28	125.08	119.28
1	D	167	ASP	N-CA-C	5.00	116.81	111.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ILE	Mainchain
1	B	137	ILE	Peptide
1	D	19	ILE	Mainchain
1	G	19	ILE	Mainchain

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	1228	0	1254	27	0
1	B	1228	0	1254	32	0
1	C	1223	0	1252	34	0
1	D	1233	0	1259	39	0
1	E	1216	0	1245	31	0
1	F	1218	0	1250	48	0
1	G	1228	0	1257	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	7	0	0	0	0
2	B	3	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
All	All	8602	0	8771	214	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 12.

All (214) 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:118:GLU:HG3	1:G:141:ARG:NH1	1.83	0.94
1:C:40:ALA:O	1:C:44:VAL:HG23	1.66	0.93
1:D:160:PRO:HD2	1:D:163:VAL:HG11	1.49	0.93
1:E:108:LYS:HG2	1:E:156:ARG:HH12	1.32	0.92
1:A:118:GLU:HG3	1:G:141:ARG:CZ	2.02	0.90
1:E:106:GLY:O	1:E:156:ARG:NH2	2.07	0.87
1:F:155:GLU:OE1	1:F:156:ARG:HD2	1.75	0.87
1:C:120:MET:SD	1:C:173:PHE:CE1	2.70	0.85
1:D:19:ILE:O	1:D:21:SER:N	2.09	0.85
1:F:140:LYS:HZ2	1:G:173:PHE:HZ	1.22	0.83
1:B:67:GLY:HA3	1:B:97:SER:HB3	1.60	0.83
1:G:40:ALA:O	1:G:44:VAL:HG23	1.79	0.83
1:E:67:GLY:HA3	1:E:97:SER:HB3	1.59	0.82
1:B:138:ALA:HB2	1:C:173:PHE:CZ	2.15	0.82
1:A:19:ILE:O	1:A:21:SER:N	2.13	0.81
1:A:67:GLY:HA3	1:A:97:SER:HB3	1.65	0.79
1:C:67:GLY:HA3	1:C:97:SER:HB3	1.64	0.78
1:G:67:GLY:HA3	1:G:97:SER:HB3	1.65	0.78
1:D:67:GLY:HA3	1:D:97:SER:HB3	1.66	0.77
1:F:67:GLY:HA3	1:F:97:SER:HB3	1.65	0.77
1:D:154:ALA:HA	1:D:164:ILE:CD1	2.15	0.76
1:F:40:ALA:O	1:F:44:VAL:HG23	1.87	0.75
1:D:40:ALA:O	1:D:44:VAL:HG23	1.87	0.74
1:G:19:ILE:O	1:G:21:SER:N	2.21	0.74
1:F:19:ILE:O	1:F:22:ARG:N	2.21	0.73
1:E:82:PHE:CE1	1:F:189:LEU:HD13	2.23	0.73
1:C:82:PHE:CZ	1:D:189:LEU:HD13	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:ALA:O	1:E:44:VAL:HG23	1.88	0.72
1:F:19:ILE:HG23	1:F:20:TYR:H	1.55	0.72
1:E:19:ILE:HG23	1:E:20:TYR:H	1.55	0.72
1:B:19:ILE:HG23	1:B:20:TYR:H	1.55	0.71
1:D:160:PRO:HD2	1:D:163:VAL:CG1	2.19	0.71
1:D:148:LYS:HE2	1:D:152:VAL:HG23	1.72	0.70
1:C:19:ILE:HG23	1:C:20:TYR:H	1.54	0.70
1:B:19:ILE:O	1:B:22:ARG:N	2.23	0.70
1:C:19:ILE:O	1:C:22:ARG:N	2.23	0.70
1:A:40:ALA:O	1:A:44:VAL:HG23	1.91	0.70
1:A:19:ILE:O	1:A:22:ARG:N	2.23	0.69
1:A:19:ILE:C	1:A:21:SER:H	2.00	0.69
1:D:19:ILE:C	1:D:21:SER:H	1.99	0.69
1:F:141:ARG:NH1	1:G:118:GLU:HG3	2.07	0.69
1:D:19:ILE:HG12	1:D:20:TYR:N	2.08	0.68
1:A:73:GLY:HA3	1:A:98:MET:HE2	1.75	0.68
1:G:73:GLY:HA3	1:G:98:MET:HE2	1.76	0.67
1:B:40:ALA:O	1:B:44:VAL:HG23	1.94	0.67
1:B:78:ASP:HB3	1:C:114:LEU:HD13	1.74	0.67
1:G:19:ILE:O	1:G:22:ARG:N	2.24	0.67
1:B:141:ARG:HG3	1:C:118:GLU:CD	2.20	0.66
1:E:19:ILE:O	1:E:22:ARG:N	2.25	0.66
1:C:120:MET:SD	1:C:173:PHE:CZ	2.89	0.66
1:C:45:SER:HB3	1:D:23:LEU:HD21	1.78	0.65
1:A:19:ILE:C	1:A:21:SER:N	2.55	0.65
1:D:19:ILE:O	1:D:22:ARG:N	2.26	0.65
1:D:154:ALA:HA	1:D:164:ILE:HD12	1.79	0.65
1:D:19:ILE:HG12	1:D:20:TYR:H	1.62	0.64
1:D:19:ILE:C	1:D:21:SER:N	2.55	0.64
1:B:141:ARG:NE	1:C:118:GLU:HG3	2.13	0.64
1:G:19:ILE:C	1:G:21:SER:H	2.06	0.64
1:D:114:LEU:HD21	1:D:189:LEU:HD12	1.81	0.63
1:E:146:ARG:HH12	1:E:168:THR:HB	1.64	0.63
1:C:73:GLY:HA3	1:C:98:MET:HE2	1.80	0.62
1:A:106:GLY:O	1:A:156:ARG:NH2	2.34	0.61
1:D:114:LEU:CD2	1:D:189:LEU:HD12	2.30	0.61
1:G:19:ILE:C	1:G:21:SER:N	2.59	0.61
1:C:82:PHE:CD1	1:D:189:LEU:HB3	2.36	0.60
1:F:166:ARG:HD2	1:F:170:ARG:HH21	1.66	0.60
1:G:139:ALA:O	1:G:143:LEU:HD23	2.02	0.59
1:E:141:ARG:NE	1:F:118:GLU:HG3	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLU:OE2	1:B:173:PHE:CD1	2.56	0.58
1:C:78:ASP:OD2	1:D:116:ASN:HB2	2.02	0.58
1:D:73:GLY:HA3	1:D:98:MET:HE2	1.85	0.57
1:B:118:GLU:OE2	1:B:173:PHE:HD1	1.87	0.57
1:A:172:ASN:C	1:A:172:ASN:OD1	2.47	0.57
1:A:121:ILE:HD11	1:A:167:ASP:HB3	1.87	0.56
1:C:19:ILE:O	1:C:21:SER:N	2.39	0.56
1:C:82:PHE:CE1	1:D:189:LEU:HB3	2.41	0.56
1:E:73:GLY:HA3	1:E:98:MET:HE2	1.88	0.56
1:D:120:MET:HE3	1:D:172:ASN:O	2.06	0.56
1:B:174:LYS:HE3	1:B:182:TYR:CD1	2.41	0.55
1:F:121:ILE:HD11	1:F:167:ASP:HB3	1.87	0.55
1:G:162:GLU:HA	1:G:162:GLU:OE1	2.05	0.55
1:F:19:ILE:O	1:F:21:SER:N	2.39	0.55
1:A:122:HIS:ND1	1:A:168:THR:O	2.35	0.55
1:G:42:SER:O	1:G:46:GLN:HG3	2.06	0.54
1:B:84:LYS:HB3	1:B:85:PRO:HD3	1.90	0.54
1:E:78:ASP:OD2	1:F:116:ASN:HB2	2.07	0.54
1:D:154:ALA:CA	1:D:164:ILE:CD1	2.85	0.54
1:C:84:LYS:HB3	1:C:85:PRO:HD3	1.90	0.54
1:E:24:LEU:HD12	1:E:50:LEU:HD21	1.89	0.54
1:D:92:ILE:O	1:D:117:SER:HB3	2.08	0.54
1:A:148:LYS:HG3	1:B:116:ASN:OD1	2.08	0.53
1:E:19:ILE:O	1:E:21:SER:N	2.40	0.53
1:D:84:LYS:HB3	1:D:85:PRO:HD3	1.91	0.53
1:B:78:ASP:HB3	1:C:114:LEU:CD1	2.39	0.53
1:F:162:GLU:CD	1:F:162:GLU:H	2.18	0.52
1:C:24:LEU:HD12	1:C:50:LEU:HD21	1.91	0.52
1:E:111:ARG:HD3	1:E:156:ARG:NH2	2.25	0.52
1:D:164:ILE:O	1:D:168:THR:HG23	2.09	0.52
1:E:84:LYS:HB3	1:E:85:PRO:HD3	1.91	0.52
1:F:73:GLY:HA3	1:F:98:MET:HE2	1.91	0.52
1:A:42:SER:O	1:A:46:GLN:HG3	2.09	0.51
1:F:174:LYS:HE2	1:F:182:TYR:CD1	2.44	0.51
1:A:84:LYS:HB3	1:A:85:PRO:HD3	1.92	0.51
1:F:123:GLN:OE1	1:F:124:PRO:C	2.54	0.51
1:A:118:GLU:OE2	1:A:173:PHE:HB2	2.09	0.51
1:B:19:ILE:O	1:B:21:SER:N	2.44	0.51
1:D:42:SER:O	1:D:46:GLN:HG3	2.12	0.50
1:C:49:PHE:O	1:C:52:ALA:HB3	2.11	0.50
1:B:73:GLY:HA3	1:B:98:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:TYR:CD1	1:C:187:LYS:HB3	2.46	0.50
1:B:49:PHE:CE1	1:C:22:ARG:CB	2.94	0.50
1:E:74:MET:HG3	1:E:145:LEU:HD22	1.93	0.49
1:D:78:ASP:HB3	1:E:114:LEU:HD13	1.94	0.49
1:E:141:ARG:CZ	1:F:118:GLU:HG3	2.42	0.49
1:B:42:SER:O	1:B:46:GLN:HG3	2.13	0.49
1:F:118:GLU:OE2	1:F:173:PHE:HB2	2.13	0.49
1:G:84:LYS:HB3	1:G:85:PRO:HD3	1.95	0.49
1:F:49:PHE:HB2	1:G:23:LEU:HD13	1.94	0.49
1:C:121:ILE:HD11	1:C:167:ASP:HB3	1.95	0.49
1:E:42:SER:O	1:E:46:GLN:HG3	2.13	0.49
1:E:92:ILE:O	1:E:117:SER:HB3	2.13	0.48
1:C:166:ARG:HE	1:C:166:ARG:HB3	1.50	0.48
1:D:154:ALA:CA	1:D:164:ILE:HD12	2.43	0.48
1:D:141:ARG:HH21	1:E:118:GLU:HG3	1.77	0.48
1:F:141:ARG:HD3	1:G:118:GLU:CD	2.38	0.48
1:F:19:ILE:C	1:F:21:SER:N	2.71	0.48
1:A:24:LEU:HD12	1:A:50:LEU:HD21	1.95	0.48
1:G:24:LEU:HD12	1:G:50:LEU:HD21	1.96	0.48
1:D:160:PRO:O	1:D:163:VAL:HG13	2.14	0.47
1:E:19:ILE:C	1:E:21:SER:N	2.70	0.47
1:F:78:ASP:HB3	1:G:114:LEU:HD13	1.96	0.47
1:F:42:SER:O	1:F:46:GLN:HG3	2.14	0.47
1:D:161:LEU:O	1:D:161:LEU:HD12	2.14	0.47
1:F:113:ALA:HB3	1:F:185:ILE:HD13	1.97	0.47
1:B:140:LYS:HB3	1:B:140:LYS:HE2	1.51	0.47
1:C:19:ILE:C	1:C:21:SER:N	2.71	0.47
1:D:160:PRO:O	1:D:163:VAL:CG1	2.63	0.47
1:C:42:SER:O	1:C:46:GLN:HG3	2.15	0.47
1:F:84:LYS:HB3	1:F:85:PRO:HD3	1.97	0.47
1:B:19:ILE:C	1:B:21:SER:N	2.74	0.46
1:A:116:ASN:HB2	1:G:78:ASP:OD2	2.16	0.46
1:G:153:LEU:HB3	1:G:164:ILE:HD12	1.97	0.46
1:D:167:ASP:OD2	1:D:182:TYR:OH	2.25	0.45
1:B:175:SER:OG	1:B:178:GLU:HG3	2.16	0.45
1:E:141:ARG:HG3	1:F:118:GLU:CD	2.42	0.45
1:G:74:MET:HG3	1:G:145:LEU:HD22	1.98	0.45
1:G:160:PRO:C	1:G:162:GLU:N	2.71	0.45
1:C:84:LYS:N	1:C:85:PRO:CD	2.79	0.45
1:G:160:PRO:O	1:G:163:VAL:HG22	2.16	0.45
1:A:78:ASP:HB3	1:B:114:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:LEU:HD12	1:F:144:LEU:HA	1.75	0.45
1:B:138:ALA:HB2	1:C:173:PHE:CE1	2.51	0.45
1:B:174:LYS:HB3	1:B:178:GLU:HB2	1.99	0.45
1:G:148:LYS:O	1:G:152:VAL:HG23	2.16	0.44
1:G:112:TYR:CD1	1:G:187:LYS:HB3	2.51	0.44
1:F:24:LEU:HD12	1:F:50:LEU:HD21	2.00	0.44
1:D:101:PHE:CZ	1:D:152:VAL:HG11	2.53	0.44
1:G:173:PHE:H	1:G:173:PHE:HD2	1.64	0.44
1:F:160:PRO:HG2	1:F:163:VAL:CG2	2.48	0.44
1:G:92:ILE:O	1:G:117:SER:HB3	2.18	0.44
1:A:101:PHE:CD1	1:A:149:LEU:HD12	2.52	0.44
1:B:19:ILE:HG23	1:B:20:TYR:N	2.30	0.44
1:F:120:MET:HE3	1:F:120:MET:HB3	1.87	0.44
1:E:144:LEU:HD12	1:E:144:LEU:HA	1.74	0.43
1:G:23:LEU:HD12	1:G:23:LEU:HA	1.83	0.43
1:F:166:ARG:CD	1:F:170:ARG:HH21	2.30	0.43
1:F:174:LYS:HE2	1:F:182:TYR:CG	2.52	0.43
1:A:92:ILE:O	1:A:117:SER:HB3	2.18	0.43
1:E:82:PHE:CD1	1:F:189:LEU:HB3	2.53	0.43
1:E:111:ARG:HD3	1:E:156:ARG:HH21	1.82	0.43
1:E:123:GLN:HB3	1:E:146:ARG:NH1	2.33	0.43
1:F:23:LEU:HD12	1:F:23:LEU:HA	1.85	0.43
1:F:152:VAL:O	1:F:156:ARG:HG2	2.17	0.43
1:B:62:TYR:CE1	1:B:90:ILE:HD13	2.54	0.43
1:A:181:GLU:OE1	1:A:181:GLU:HA	2.19	0.43
1:F:30:MET:HE2	1:F:30:MET:HB2	1.78	0.43
1:F:172:ASN:ND2	1:F:172:ASN:C	2.76	0.43
1:D:148:LYS:HA	1:D:148:LYS:HD2	1.79	0.43
1:F:19:ILE:HG23	1:F:20:TYR:CD2	2.54	0.43
1:B:138:ALA:HB2	1:C:173:PHE:CE2	2.54	0.42
1:D:157:THR:HB	1:D:159:GLN:HG2	1.99	0.42
1:F:159:GLN:HB2	1:F:164:ILE:HD11	2.01	0.42
1:B:141:ARG:HE	1:C:118:GLU:HG3	1.82	0.42
1:F:20:TYR:HA	1:F:23:LEU:HB2	2.02	0.42
1:C:92:ILE:O	1:C:117:SER:HB3	2.20	0.42
1:G:174:LYS:HZ3	1:G:174:LYS:HG3	1.73	0.42
1:D:159:GLN:HA	1:D:160:PRO:HD3	1.93	0.42
1:A:114:LEU:HD13	1:G:78:ASP:HB3	2.01	0.42
1:C:44:VAL:HG13	1:C:79:THR:OG1	2.20	0.42
1:A:19:ILE:HG12	1:A:20:TYR:N	2.35	0.41
1:E:19:ILE:HG23	1:E:20:TYR:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:GLY:O	1:F:156:ARG:NH2	2.53	0.41
1:G:62:TYR:CE1	1:G:90:ILE:HD13	2.55	0.41
1:G:121:ILE:HD11	1:G:167:ASP:HB3	2.02	0.41
1:C:112:TYR:HD1	1:C:187:LYS:HB3	1.85	0.41
1:E:19:ILE:HG23	1:E:20:TYR:CD2	2.55	0.41
1:F:119:VAL:HG11	1:F:184:LEU:HD13	2.02	0.41
1:G:141:ARG:CZ	1:G:145:LEU:HD11	2.50	0.41
1:F:141:ARG:CZ	1:G:118:GLU:HG3	2.49	0.41
1:A:156:ARG:HA	1:A:156:ARG:HD2	1.76	0.41
1:G:142:ILE:H	1:G:142:ILE:HG13	1.55	0.41
1:B:144:LEU:HD12	1:B:144:LEU:HA	1.83	0.41
1:F:160:PRO:HG2	1:F:163:VAL:HG23	2.02	0.41
1:D:84:LYS:N	1:D:85:PRO:CD	2.84	0.41
1:B:23:LEU:HD12	1:B:23:LEU:HA	1.91	0.41
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.83	0.41
1:B:157:THR:OG1	1:B:159:GLN:HB2	2.21	0.41
1:E:23:LEU:HD12	1:E:23:LEU:HA	1.88	0.41
1:F:19:ILE:HG23	1:F:20:TYR:N	2.31	0.41
1:E:145:LEU:HA	1:E:145:LEU:HD23	1.82	0.40
1:G:174:LYS:HE3	1:G:182:TYR:CD1	2.56	0.40
1:B:123:GLN:OE1	1:B:124:PRO:HD2	2.21	0.40
1:F:140:LYS:NZ	1:G:173:PHE:HZ	2.04	0.40
1:F:39:VAL:O	1:F:43:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

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	158/196 (81%)	155 (98%)	2 (1%)	1 (1%)	21 42
1	B	158/196 (81%)	154 (98%)	3 (2%)	1 (1%)	21 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	157/196 (80%)	152 (97%)	3 (2%)	2 (1%)	9	21
1	D	158/196 (81%)	155 (98%)	2 (1%)	1 (1%)	21	42
1	E	156/196 (80%)	151 (97%)	4 (3%)	1 (1%)	21	42
1	F	156/196 (80%)	152 (97%)	3 (2%)	1 (1%)	21	42
1	G	157/196 (80%)	152 (97%)	4 (2%)	1 (1%)	21	42
All	All	1100/1372 (80%)	1071 (97%)	21 (2%)	8 (1%)	18	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	C	137	ILE
1	D	20	TYR
1	G	20	TYR
1	B	20	TYR
1	C	20	TYR
1	E	20	TYR
1	F	20	TYR

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	130/162 (80%)	115 (88%)	15 (12%)	5	11
1	B	130/162 (80%)	116 (89%)	14 (11%)	6	13
1	C	130/162 (80%)	119 (92%)	11 (8%)	10	22
1	D	131/162 (81%)	115 (88%)	16 (12%)	5	10
1	E	129/162 (80%)	119 (92%)	10 (8%)	11	26
1	F	130/162 (80%)	117 (90%)	13 (10%)	7	16
1	G	131/162 (81%)	116 (88%)	15 (12%)	5	11
All	All	911/1134 (80%)	817 (90%)	94 (10%)	7	15

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	21	SER
1	A	23	LEU
1	A	24	LEU
1	A	28	ILE
1	A	69	SER
1	A	120	MET
1	A	141	ARG
1	A	144	LEU
1	A	146	ARG
1	A	148	LYS
1	A	149	LEU
1	A	155	GLU
1	A	166	ARG
1	A	169	ASP
1	B	19	ILE
1	B	21	SER
1	B	23	LEU
1	B	24	LEU
1	B	28	ILE
1	B	69	SER
1	B	140	LYS
1	B	143	LEU
1	B	144	LEU
1	B	146	ARG
1	B	148	LYS
1	B	162	GLU
1	B	172	ASN
1	B	187	LYS
1	C	19	ILE
1	C	21	SER
1	C	23	LEU
1	C	24	LEU
1	C	28	ILE
1	C	69	SER
1	C	120	MET
1	C	146	ARG
1	C	162	GLU
1	C	166	ARG
1	C	171	ASP
1	D	19	ILE
1	D	21	SER

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Mol	Chain	Res	Type
1	D	23	LEU
1	D	24	LEU
1	D	28	ILE
1	D	69	SER
1	D	92	ILE
1	D	120	MET
1	D	141	ARG
1	D	143	LEU
1	D	144	LEU
1	D	146	ARG
1	D	155	GLU
1	D	157	THR
1	D	163	VAL
1	D	170	ARG
1	E	19	ILE
1	E	21	SER
1	E	23	LEU
1	E	24	LEU
1	E	28	ILE
1	E	69	SER
1	E	120	MET
1	E	144	LEU
1	E	162	GLU
1	E	166	ARG
1	F	19	ILE
1	F	21	SER
1	F	23	LEU
1	F	24	LEU
1	F	28	ILE
1	F	69	SER
1	F	92	ILE
1	F	120	MET
1	F	141	ARG
1	F	144	LEU
1	F	162	GLU
1	F	166	ARG
1	F	170	ARG
1	G	19	ILE
1	G	21	SER
1	G	23	LEU
1	G	24	LEU
1	G	28	ILE

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Mol	Chain	Res	Type
1	G	69	SER
1	G	120	MET
1	G	141	ARG
1	G	144	LEU
1	G	146	ARG
1	G	151	LYS
1	G	170	ARG
1	G	173	PHE
1	G	174	LYS
1	G	190	THR

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	46	GLN
1	B	46	GLN
1	C	172	ASN
1	D	41	ASN
1	D	191	HIS
1	E	46	GLN
1	F	46	GLN
1	F	172	ASN
1	G	46	GLN
1	G	172	ASN

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(Å ²)	Q<0.9
1	A	162/196 (82%)	0.24	7 (4%) 40 34	47, 62, 96, 112	0
1	B	162/196 (82%)	0.34	9 (5%) 30 24	50, 65, 96, 121	0
1	C	161/196 (82%)	0.18	5 (3%) 51 45	41, 63, 95, 115	0
1	D	162/196 (82%)	0.23	4 (2%) 58 52	49, 68, 101, 124	0
1	E	160/196 (81%)	0.14	8 (5%) 34 28	44, 61, 96, 113	0
1	F	160/196 (81%)	0.20	5 (3%) 51 45	49, 64, 95, 114	0
1	G	161/196 (82%)	0.33	3 (1%) 66 61	51, 72, 102, 114	0
All	All	1128/1372 (82%)	0.24	41 (3%) 46 40	41, 65, 99, 124	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	ILE	4.5
1	D	19	ILE	4.4
1	A	191	HIS	4.2
1	A	123	GLN	4.1
1	F	19	ILE	4.0
1	G	19	ILE	3.9
1	E	19	ILE	3.6
1	B	191	HIS	3.6
1	A	19	ILE	3.5
1	C	124	PRO	3.3
1	C	82	PHE	3.1
1	C	19	ILE	3.1
1	E	82	PHE	2.9
1	E	138	ALA	2.8
1	E	136	GLU	2.8
1	E	137	ILE	2.8
1	C	137	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	118	GLU	2.6
1	D	136	GLU	2.6
1	E	123	GLN	2.5
1	E	30	MET	2.4
1	D	20	TYR	2.4
1	A	172	ASN	2.3
1	A	137	ILE	2.3
1	B	30	MET	2.3
1	F	171	ASP	2.3
1	E	120	MET	2.2
1	C	173	PHE	2.2
1	A	124	PRO	2.2
1	B	20	TYR	2.2
1	B	136	GLU	2.2
1	G	101	PHE	2.2
1	A	82	PHE	2.2
1	B	82	PHE	2.2
1	F	191	HIS	2.1
1	B	92	ILE	2.1
1	F	169	ASP	2.1
1	F	138	ALA	2.1
1	D	137	ILE	2.1
1	G	20	TYR	2.0
1	B	57	LYS	2.0

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.