



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:12 am BST

PDB ID : 1DR0
Title : STRUCTURE OF MODIFIED 3-ISOPROPYLMALATE DEHYDROGENASE AT THE C-TERMINUS, HD708
Authors : Nurachman, Z.; Akanuma, S.; Sato, T.; Oshima, T.; Tanaka, N.
Deposited on : 2000-01-06
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

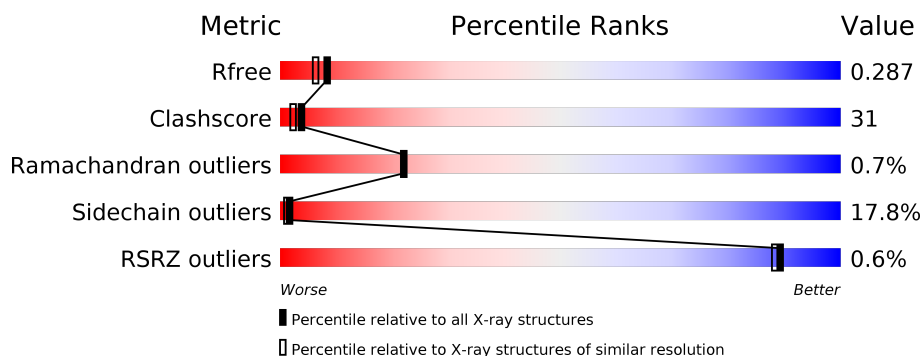
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	346	
1	B	346	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5331 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 3-ISOPROPYLMALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2594	1654	448	486	6			
1	B	346	Total	C	N	O	S	0	0	0
			2594	1654	448	486	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ARG	SER	see remark 999	UNP Q5SIY4
A	172	LEU	ALA	see remark 999	UNP Q5SIY4
A	341	THR	LEU	see remark 999	UNP Q5SIY4
A	342	ALA	ARG	see remark 999	UNP Q5SIY4
A	343	THR	HIS	see remark 999	UNP Q5SIY4
A	344	VAL	LEU	see remark 999	UNP Q5SIY4
A	345	GLY	ALA	see remark 999	UNP Q5SIY4
A	346	ILE	-	see remark 999	UNP Q5SIY4
B	85	ARG	SER	see remark 999	UNP Q5SIY4
B	172	LEU	ALA	see remark 999	UNP Q5SIY4
B	341	THR	LEU	see remark 999	UNP Q5SIY4
B	342	ALA	ARG	see remark 999	UNP Q5SIY4
B	343	THR	HIS	see remark 999	UNP Q5SIY4
B	344	VAL	LEU	see remark 999	UNP Q5SIY4
B	345	GLY	ALA	see remark 999	UNP Q5SIY4
B	346	ILE	-	see remark 999	UNP Q5SIY4

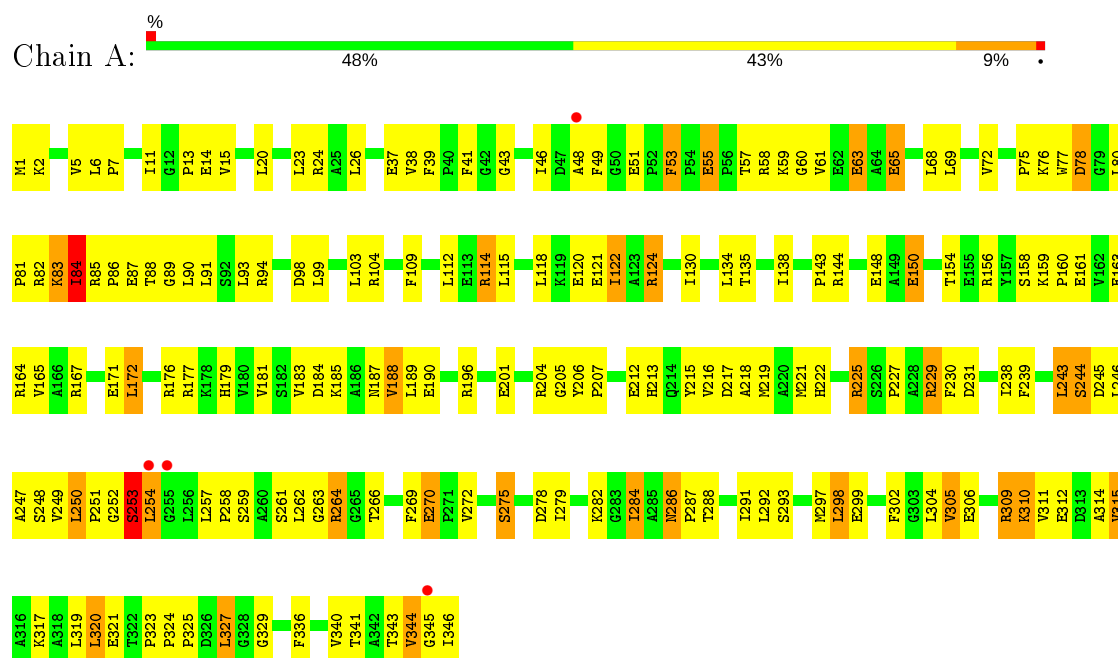
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	B	78	Total	O	0	0
			78	78		

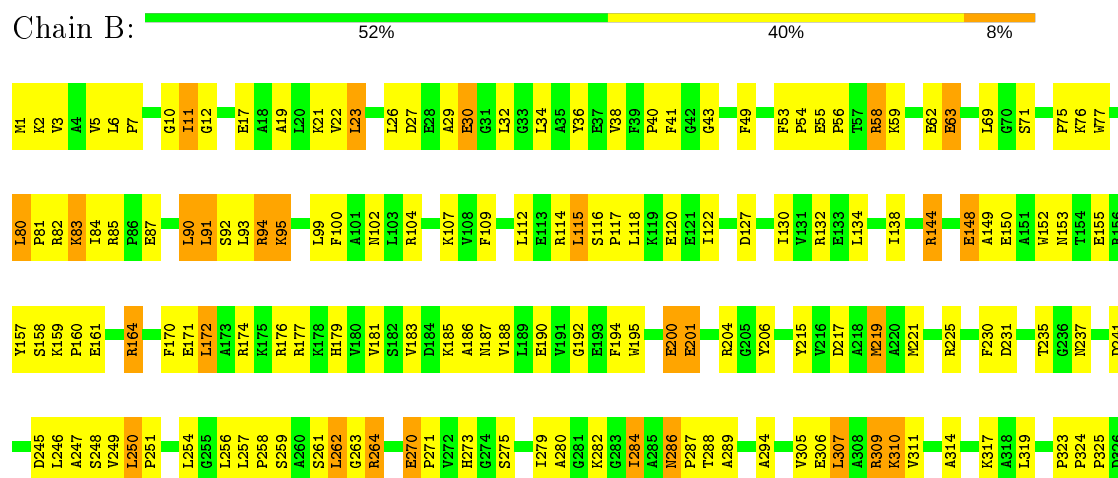
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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: 3-ISOPROPYLMALATE DEHYDROGENASE



- Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE



I327	G328	G329	F336	T337	V340	T341	A342	T343	V344	G345	I346
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.62Å 84.31Å 72.28Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	7.99 – 2.20 54.19 – 1.79	Depositor EDS
% Data completeness (in resolution range)	85.6 (7.99-2.20) 64.5 (54.19-1.79)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.80Å)	Xtriage
Refinement program	X-PLOR (ONLINE) 98.1	Depositor
R, R_{free}	0.249 , 0.308 0.231 , 0.287	Depositor DCC
R_{free} test set	3945 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5331	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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 [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	0.53	0/2648	0.72	0/3595
1	B	0.55	0/2648	0.73	1/3595 (0.0%)
All	All	0.54	0/5296	0.72	1/7190 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	LEU	CA-CB-CG	5.95	128.99	115.30

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	2594	0	2634	180	0
1	B	2594	0	2634	155	0
2	A	65	0	0	5	1
2	B	78	0	0	8	1
All	All	5331	0	5268	323	1

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 31.

All (323) 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:309:ARG:HH11	1:A:309:ARG:HG3	1.06	1.12
1:B:81:PRO:HD2	1:B:84:ILE:HD11	1.34	1.06
1:B:94:ARG:HG3	2:B:383:HOH:O	1.58	1.03
1:A:94:ARG:HD2	2:A:377:HOH:O	1.61	1.01
1:A:94:ARG:HD3	1:A:134:LEU:HD13	1.44	0.97
1:B:254:LEU:HD12	1:B:257:LEU:HD12	1.47	0.94
1:A:309:ARG:NH1	1:A:309:ARG:HG3	1.78	0.93
1:B:82:ARG:HG2	1:B:85:ARG:HH22	1.35	0.92
1:A:135:THR:HG21	1:A:164:ARG:HH21	1.38	0.87
1:A:82:ARG:HH22	1:A:87:GLU:HB2	1.39	0.86
1:B:342:ALA:O	1:B:346:ILE:HG13	1.76	0.85
1:A:82:ARG:NH2	1:A:87:GLU:HB2	1.94	0.83
1:A:311:VAL:O	1:A:315:VAL:HG12	1.79	0.83
1:B:27:ASP:HA	1:B:32:LEU:HG	1.61	0.82
1:B:251:PRO:HG2	1:B:257:LEU:HD21	1.61	0.82
1:A:185:LYS:HG3	1:A:188:VAL:HG12	1.61	0.81
1:B:23:LEU:HD21	1:B:294:ALA:HB1	1.61	0.81
1:B:341:THR:O	1:B:344:VAL:HG22	1.82	0.80
1:B:179:HIS:HB2	2:B:352:HOH:O	1.81	0.80
1:A:187:ASN:HB3	1:A:215:TYR:CZ	2.17	0.80
1:B:200:GLU:HG3	2:B:347:HOH:O	1.80	0.79
1:B:340:VAL:O	1:B:344:VAL:HG13	1.82	0.78
1:A:309:ARG:CG	1:A:309:ARG:HH11	1.91	0.78
1:A:135:THR:HG21	1:A:164:ARG:NH2	1.98	0.77
1:B:82:ARG:HG2	1:B:85:ARG:NH2	1.98	0.77
1:B:1:MET:SD	1:B:32:LEU:HD13	2.26	0.76
1:A:84:ILE:HG12	1:A:84:ILE:O	1.83	0.76
1:A:122:ILE:HD12	1:A:227:PRO:HD2	1.68	0.76
1:B:176:ARG:NH1	1:B:231:ASP:OD1	2.19	0.75
1:A:124:ARG:HD3	2:A:368:HOH:O	1.86	0.75
1:A:254:LEU:H	1:A:254:LEU:HD22	1.52	0.75
1:B:286:ASN:ND2	1:B:288:THR:H	1.84	0.75
1:A:310:LYS:NZ	1:A:344:VAL:O	2.19	0.75
1:A:94:ARG:HG3	1:A:99:LEU:HB2	1.68	0.74
1:B:132:ARG:NH1	1:B:237:ASN:OD1	2.21	0.74
1:A:247:ALA:HA	1:A:250:LEU:HD22	1.69	0.73
1:A:55:GLU:HA	1:A:58:ARG:NH1	2.02	0.73
1:B:69:LEU:HD21	1:B:90:LEU:HD21	1.71	0.73
1:A:183:VAL:HG21	1:A:219:MET:HG2	1.68	0.73
1:A:75:PRO:HA	1:A:78:ASP:OD2	1.88	0.72
1:A:179:HIS:NE2	1:A:181:VAL:HG22	2.04	0.72
1:A:317:LYS:HE2	1:A:343:THR:HG23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:HA	1:A:99:LEU:HD12	1.73	0.70
1:B:19:ALA:O	1:B:23:LEU:HD22	1.92	0.70
1:B:83:LYS:HG3	1:B:84:ILE:HG23	1.73	0.69
1:A:55:GLU:HB2	1:A:58:ARG:HH12	1.58	0.69
1:A:46:ILE:HD11	1:A:86:PRO:HD3	1.76	0.68
1:A:254:LEU:HD13	1:A:254:LEU:N	2.09	0.68
1:B:80:LEU:HD23	2:B:413:HOH:O	1.94	0.67
1:A:72:VAL:HG13	1:A:86:PRO:HB3	1.77	0.66
1:B:246:LEU:O	1:B:249:VAL:HG22	1.94	0.66
1:A:122:ILE:CD1	1:A:227:PRO:HD2	2.25	0.66
1:A:143:PRO:O	1:A:154:THR:HG23	1.94	0.66
1:B:32:LEU:HD11	1:B:34:LEU:HB2	1.77	0.66
1:B:11:ILE:HD11	1:B:273:HIS:CE1	2.30	0.65
1:B:91:LEU:HD12	1:B:95:LYS:HE2	1.77	0.65
1:A:143:PRO:HD2	1:A:154:THR:HG21	1.77	0.65
1:B:325:PRO:HG2	2:B:380:HOH:O	1.97	0.65
1:B:69:LEU:HD23	1:B:270:GLU:CD	2.18	0.65
1:A:225:ARG:HD2	2:A:398:HOH:O	1.96	0.64
1:A:43:GLY:HA2	1:A:46:ILE:HD12	1.79	0.64
1:B:53:PHE:CE2	1:B:58:ARG:HG3	2.32	0.64
1:B:80:LEU:HB3	1:B:84:ILE:CD1	2.26	0.64
1:A:37:GLU:HB3	1:A:39:PHE:CE1	2.32	0.64
1:A:53:PHE:CE2	1:A:93:LEU:HA	2.33	0.63
1:A:55:GLU:HA	1:A:58:ARG:CZ	2.27	0.63
1:A:2:LYS:H	1:A:65:GLU:HG3	1.64	0.63
1:A:181:VAL:HG21	1:A:230:PHE:HD1	1.63	0.63
1:A:75:PRO:O	1:A:78:ASP:OD1	2.17	0.63
1:B:159:LYS:HB3	1:B:160:PRO:HD3	1.79	0.63
1:B:306:GLU:O	1:B:310:LYS:HD3	1.99	0.63
1:A:341:THR:O	1:A:344:VAL:HG12	1.98	0.62
1:B:76:LYS:HD3	1:B:77:TRP:CZ2	2.34	0.62
1:B:2:LYS:HD2	1:B:63:GLU:O	2.00	0.62
1:B:26:LEU:HD21	1:B:311:VAL:HG22	1.82	0.62
1:B:286:ASN:HD22	1:B:286:ASN:C	2.02	0.62
1:A:185:LYS:HG3	1:A:188:VAL:CG1	2.30	0.61
1:B:69:LEU:HD23	1:B:270:GLU:OE2	1.99	0.61
1:B:80:LEU:HB3	1:B:84:ILE:HD11	1.80	0.61
1:A:39:PHE:HB3	1:A:57:THR:OG1	2.00	0.61
1:B:99:LEU:HD22	1:B:261:SER:O	2.00	0.61
1:A:284:ILE:HG22	1:A:325:PRO:HG2	1.83	0.61
1:A:201:GLU:O	1:A:204:ARG:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD11	1:B:138:ILE:HD13	1.83	0.60
1:B:200:GLU:CG	2:B:347:HOH:O	2.44	0.60
1:B:21:LYS:HD3	1:B:337:THR:HG21	1.82	0.59
1:A:254:LEU:HD12	2:A:396:HOH:O	2.02	0.59
1:B:94:ARG:HA	1:B:99:LEU:HD12	1.83	0.59
1:A:196:ARG:CZ	1:A:213:HIS:HB3	2.33	0.59
1:A:187:ASN:HB3	1:A:215:TYR:OH	2.03	0.58
1:A:217:ASP:HB2	1:B:245:ASP:OD2	2.04	0.58
1:A:314:ALA:HA	1:A:343:THR:CG2	2.34	0.58
1:A:11:ILE:HG12	1:A:275:SER:O	2.04	0.57
1:A:7:PRO:HB3	1:A:13:PRO:HA	1.86	0.57
1:A:98:ASP:OD2	1:A:264:ARG:HG3	2.04	0.57
1:B:286:ASN:HD22	1:B:288:THR:H	1.51	0.57
1:B:204:ARG:HG2	1:B:204:ARG:HH11	1.68	0.57
1:B:256:LEU:O	1:B:258:PRO:HD3	2.05	0.57
1:B:11:ILE:HG22	1:B:280:ALA:HA	1.86	0.57
1:A:181:VAL:HG21	1:A:230:PHE:CD1	2.39	0.56
1:A:39:PHE:CE2	1:A:60:GLY:HA3	2.40	0.56
1:B:171:GLU:O	1:B:174:ARG:HB2	2.05	0.56
1:A:150:GLU:HB3	1:B:158:SER:HA	1.86	0.56
1:B:248:SER:HB2	1:B:257:LEU:HD13	1.86	0.56
1:A:82:ARG:HD2	1:A:85:ARG:HH22	1.71	0.56
1:A:286:ASN:ND2	1:A:288:THR:H	2.03	0.56
1:A:216:VAL:HG13	1:A:217:ASP:N	2.21	0.56
1:A:246:LEU:O	1:A:249:VAL:HG22	2.05	0.56
1:A:319:LEU:HG	1:A:336:PHE:HZ	1.71	0.55
1:B:114:ARG:HG3	1:B:115:LEU:N	2.21	0.55
1:B:116:SER:OG	1:B:117:PRO:HD2	2.06	0.55
1:B:112:LEU:HD22	1:B:115:LEU:HD22	1.88	0.55
1:B:148:GLU:HG3	1:B:149:ALA:N	2.21	0.54
1:A:184:ASP:OD2	1:A:196:ARG:HD2	2.07	0.54
1:A:286:ASN:HD22	1:A:287:PRO:HD2	1.72	0.54
1:A:53:PHE:HE1	1:A:57:THR:HG22	1.71	0.54
1:B:187:ASN:HB3	1:B:215:TYR:CZ	2.43	0.54
1:A:287:PRO:O	1:A:291:ILE:HG13	2.08	0.54
1:B:27:ASP:CA	1:B:32:LEU:HG	2.35	0.54
1:A:176:ARG:HD3	1:A:231:ASP:OD1	2.09	0.53
1:B:40:PRO:HG3	1:B:49:PHE:CE1	2.43	0.53
1:A:258:PRO:HG3	1:A:292:LEU:HB3	1.88	0.53
1:A:48:ALA:O	1:A:49:PHE:CG	2.62	0.53
1:B:271:PRO:HB3	1:B:289:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:O	1:A:315:VAL:HG13	2.09	0.53
1:A:6:LEU:HD23	1:A:41:PHE:CG	2.44	0.53
1:A:80:LEU:HB3	1:A:81:PRO:HD2	1.91	0.53
1:B:53:PHE:CZ	1:B:58:ARG:HG3	2.43	0.52
1:A:159:LYS:N	1:A:160:PRO:HD2	2.23	0.52
1:A:65:GLU:HB2	1:A:302:PHE:CE1	2.45	0.52
1:B:314:ALA:HA	1:B:343:THR:HG21	1.92	0.52
1:A:81:PRO:HG2	1:A:84:ILE:CG2	2.40	0.52
1:A:2:LYS:H	1:A:65:GLU:CG	2.23	0.51
1:A:317:LYS:HB3	1:A:343:THR:HG21	1.91	0.51
1:B:69:LEU:O	1:B:270:GLU:HB2	2.11	0.51
1:B:132:ARG:HD2	1:B:237:ASN:O	2.11	0.51
1:B:286:ASN:HD22	1:B:287:PRO:N	2.07	0.51
1:B:69:LEU:CD2	1:B:90:LEU:HD21	2.40	0.51
1:A:5:VAL:HG12	1:A:7:PRO:HD3	1.92	0.51
1:B:54:PRO:HB2	1:B:56:PRO:HD2	1.92	0.51
1:B:107:LYS:HD2	1:B:109:PHE:CE1	2.46	0.50
1:B:144:ARG:HB3	1:B:153:ASN:HD22	1.76	0.50
1:B:58:ARG:O	1:B:62:GLU:HG2	2.12	0.50
1:B:115:LEU:HD21	1:B:327:LEU:HD13	1.92	0.50
1:A:88:THR:O	1:A:91:LEU:HB3	2.11	0.50
1:A:11:ILE:O	1:A:15:VAL:HG22	2.12	0.50
1:B:77:TRP:HA	1:B:80:LEU:CD2	2.42	0.50
1:B:5:VAL:O	1:B:7:PRO:HD3	2.12	0.50
1:B:195:TRP:CZ2	1:B:235:THR:HA	2.47	0.49
1:B:314:ALA:HA	1:B:343:THR:CG2	2.42	0.49
1:A:11:ILE:O	1:A:14:GLU:HG2	2.12	0.49
1:A:55:GLU:CA	1:A:58:ARG:NH1	2.74	0.49
1:B:116:SER:OG	1:B:250:LEU:O	2.18	0.49
1:A:206:TYR:N	1:A:207:PRO:HD3	2.26	0.49
1:A:2:LYS:N	1:A:65:GLU:HG3	2.26	0.49
1:B:5:VAL:C	1:B:6:LEU:HD12	2.32	0.49
1:A:323:PRO:O	1:A:329:GLY:HA3	2.13	0.49
1:A:55:GLU:HB2	1:A:58:ARG:NH1	2.25	0.49
1:A:80:LEU:HB2	1:A:85:ARG:HG2	1.94	0.49
1:A:249:VAL:HG13	1:B:221:MET:HG2	1.93	0.49
1:A:2:LYS:HB3	1:A:65:GLU:HG2	1.94	0.49
1:A:286:ASN:HD22	1:A:287:PRO:CD	2.26	0.48
1:A:314:ALA:HA	1:A:343:THR:HG22	1.95	0.48
1:A:53:PHE:HE2	1:A:93:LEU:HA	1.77	0.48
1:A:76:LYS:HD3	1:A:77:TRP:CZ2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ARG:HB3	1:A:177:ARG:H	1.49	0.48
1:A:221:MET:CE	1:A:225:ARG:HH12	2.26	0.48
1:A:99:LEU:HA	1:A:263:GLY:HA3	1.94	0.48
1:B:99:LEU:HA	1:B:263:GLY:HA3	1.94	0.48
1:B:186:ALA:HB2	1:B:192:GLY:O	2.14	0.48
1:B:323:PRO:HA	1:B:324:PRO:HD3	1.64	0.48
1:A:112:LEU:HD13	1:A:320:LEU:HD11	1.95	0.48
1:B:23:LEU:HD21	1:B:294:ALA:CB	2.40	0.48
1:B:247:ALA:O	1:B:250:LEU:HB2	2.12	0.48
1:B:82:ARG:HA	1:B:85:ARG:CZ	2.43	0.48
1:A:317:LYS:O	1:A:321:GLU:HG3	2.14	0.48
1:B:43:GLY:HA3	1:B:77:TRP:CE2	2.49	0.48
1:A:58:ARG:O	1:A:61:VAL:HG22	2.14	0.48
1:A:81:PRO:HG2	1:A:84:ILE:HG21	1.95	0.48
1:B:264:ARG:NH1	1:B:264:ARG:HG2	2.29	0.48
1:A:238:ILE:HG23	1:A:239:PHE:N	2.28	0.48
1:A:254:LEU:HD11	1:B:225:ARG:HH12	1.79	0.47
1:A:257:LEU:O	1:A:272:VAL:HG23	2.13	0.47
1:A:336:PHE:O	1:A:340:VAL:HG23	2.14	0.47
1:B:11:ILE:HD13	1:B:11:ILE:C	2.34	0.47
1:A:317:LYS:HE2	1:A:343:THR:CG2	2.42	0.47
1:A:5:VAL:C	1:A:6:LEU:HD12	2.35	0.47
1:B:112:LEU:HD11	1:B:319:LEU:HB3	1.96	0.47
1:A:314:ALA:HA	1:A:343:THR:HG21	1.96	0.47
1:A:46:ILE:CD1	1:A:86:PRO:HD3	2.43	0.47
1:B:102:ASN:HB2	1:B:134:LEU:HD21	1.96	0.47
1:B:160:PRO:O	1:B:164:ARG:HG2	2.15	0.47
1:A:55:GLU:CA	1:A:58:ARG:CZ	2.92	0.47
1:A:83:LYS:CD	1:A:83:LYS:N	2.77	0.47
1:B:342:ALA:O	1:B:346:ILE:CG1	2.58	0.47
1:B:82:ARG:HA	1:B:85:ARG:NH1	2.30	0.47
1:A:103:LEU:HD21	1:A:172:LEU:HD21	1.97	0.47
1:A:183:VAL:CG2	1:A:219:MET:HG2	2.40	0.47
1:A:218:ALA:O	1:A:222:HIS:CD2	2.68	0.47
1:B:3:VAL:O	1:B:36:TYR:HB2	2.15	0.47
1:A:115:LEU:HD13	1:A:327:LEU:HD11	1.97	0.46
1:A:80:LEU:O	1:A:85:ARG:HD3	2.15	0.46
1:A:310:LYS:HE3	1:A:344:VAL:HG22	1.96	0.46
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.79	0.46
1:B:11:ILE:HD11	1:B:273:HIS:HE1	1.81	0.46
1:B:90:LEU:HD12	1:B:94:ARG:NE	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLY:C	1:A:207:PRO:HD3	2.36	0.46
1:B:307:LEU:O	1:B:310:LYS:HB2	2.16	0.46
1:A:323:PRO:HA	1:A:324:PRO:HD3	1.76	0.46
1:B:336:PHE:O	1:B:340:VAL:HG23	2.16	0.46
1:A:69:LEU:HB3	1:A:270:GLU:HB2	1.98	0.45
1:A:278:ASP:O	1:A:282:LYS:HE3	2.16	0.45
1:A:216:VAL:CG1	1:A:217:ASP:N	2.80	0.45
1:B:17:GLU:O	1:B:21:LYS:HG3	2.16	0.45
1:B:76:LYS:HD3	1:B:77:TRP:CE2	2.51	0.45
1:A:158:SER:HA	1:B:150:GLU:HB3	1.98	0.45
1:B:170:PHE:HB3	1:B:206:TYR:CD2	2.51	0.45
1:B:32:LEU:CD1	1:B:34:LEU:HB2	2.43	0.45
1:A:179:HIS:CE1	1:A:181:VAL:HG22	2.51	0.45
1:B:161:GLU:O	1:B:164:ARG:HG3	2.16	0.45
1:A:57:THR:O	1:A:61:VAL:HG13	2.17	0.45
1:A:99:LEU:HD22	1:A:261:SER:O	2.17	0.45
1:A:244:SER:O	1:A:248:SER:HB3	2.17	0.45
1:A:254:LEU:N	1:A:254:LEU:CD1	2.78	0.45
1:A:6:LEU:O	1:A:69:LEU:HD12	2.17	0.45
1:A:171:GLU:HG3	2:A:389:HOH:O	2.16	0.45
1:A:83:LYS:HD2	1:A:83:LYS:N	2.31	0.45
1:A:85:ARG:O	1:A:88:THR:HB	2.17	0.45
1:B:271:PRO:HB3	1:B:289:ALA:CB	2.47	0.45
1:A:144:ARG:HB2	1:B:190:GLU:OE2	2.17	0.44
1:B:1:MET:SD	1:B:32:LEU:CD1	3.03	0.44
1:B:282:LYS:HB2	1:B:284:ILE:HD11	1.99	0.44
1:A:344:VAL:CG1	1:A:345:GLY:N	2.80	0.44
1:A:269:PHE:CE2	1:A:297:MET:HA	2.53	0.44
1:A:305:VAL:HG12	1:A:306:GLU:N	2.32	0.44
1:B:286:ASN:ND2	1:B:286:ASN:C	2.70	0.44
1:A:189:LEU:CD1	1:B:138:ILE:HD13	2.48	0.44
1:A:20:LEU:O	1:A:24:ARG:HG3	2.18	0.44
1:B:21:LYS:CD	1:B:337:THR:HG21	2.48	0.43
1:A:344:VAL:HG12	1:A:345:GLY:N	2.33	0.43
1:A:48:ALA:C	1:A:49:PHE:CG	2.92	0.43
1:B:204:ARG:HH11	1:B:204:ARG:CG	2.31	0.43
1:B:10:GLY:HA3	1:B:275:SER:HB3	2.00	0.43
1:A:48:ALA:C	1:A:49:PHE:CD2	2.92	0.43
1:B:323:PRO:O	1:B:329:GLY:HA3	2.17	0.43
1:A:75:PRO:HA	1:A:78:ASP:CG	2.38	0.43
1:A:72:VAL:CG1	1:A:86:PRO:HB3	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:HD22	1:A:287:PRO:N	2.16	0.43
1:B:112:LEU:HD22	1:B:115:LEU:CD2	2.48	0.43
1:B:152:TRP:CE3	1:B:152:TRP:N	2.86	0.43
1:B:115:LEU:HG	1:B:327:LEU:HD22	2.00	0.43
1:A:121:GLU:HG2	1:A:122:ILE:HG22	2.01	0.43
1:A:158:SER:OG	1:A:161:GLU:HG3	2.19	0.43
1:A:279:ILE:HA	1:A:282:LYS:HE3	1.99	0.43
1:A:221:MET:HG2	1:B:245:ASP:O	2.18	0.43
1:B:309:ARG:HD2	1:B:309:ARG:N	2.33	0.43
1:A:221:MET:HE2	1:A:225:ARG:HH12	1.84	0.43
1:B:204:ARG:CZ	1:B:204:ARG:HB3	2.49	0.43
1:B:29:ALA:HB2	2:B:355:HOH:O	2.19	0.43
1:A:245:ASP:OD2	1:B:217:ASP:HB2	2.18	0.43
1:B:53:PHE:HB3	1:B:58:ARG:HH11	1.84	0.43
1:A:325:PRO:HA	1:A:329:GLY:O	2.18	0.43
1:A:82:ARG:O	1:A:88:THR:OG1	2.24	0.43
1:A:250:LEU:HB2	1:A:251:PRO:HD3	2.00	0.43
1:B:176:ARG:NH1	1:B:231:ASP:CG	2.72	0.43
1:B:26:LEU:O	1:B:30:GLU:HB2	2.19	0.43
1:A:185:LYS:HA	1:A:185:LYS:HD2	1.91	0.42
1:B:100:PHE:CD1	1:B:164:ARG:HD3	2.54	0.42
1:A:286:ASN:HD22	1:A:286:ASN:C	2.22	0.42
1:B:11:ILE:HG21	1:B:279:ILE:HD11	2.00	0.42
1:A:83:LYS:H	1:A:83:LYS:CD	2.32	0.42
1:B:112:LEU:HA	1:B:112:LEU:HD23	1.80	0.42
1:B:144:ARG:HB3	1:B:153:ASN:ND2	2.33	0.42
1:B:183:VAL:HG21	1:B:219:MET:HG3	2.00	0.42
1:B:41:PHE:CD2	1:B:69:LEU:HD11	2.54	0.42
1:A:55:GLU:N	1:A:58:ARG:NH2	2.68	0.42
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.84	0.42
1:B:5:VAL:C	1:B:7:PRO:HD3	2.40	0.42
1:A:11:ILE:HA	1:A:14:GLU:OE2	2.20	0.42
1:A:212:GLU:OE2	1:A:229:ARG:NH2	2.53	0.42
1:B:177:ARG:HB2	1:B:231:ASP:CG	2.40	0.42
1:A:114:ARG:HG2	1:A:115:LEU:N	2.35	0.42
1:B:264:ARG:HH11	1:B:264:ARG:CG	2.32	0.42
1:B:11:ILE:HD13	1:B:12:GLY:N	2.34	0.42
1:B:91:LEU:O	1:B:95:LYS:HD3	2.18	0.42
1:B:138:ILE:N	1:B:155:GLU:OE1	2.50	0.42
1:A:201:GLU:HG2	1:A:204:ARG:HH12	1.84	0.41
1:B:100:PHE:CD2	1:B:164:ARG:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PRO:HD2	2:B:388:HOH:O	2.20	0.41
1:A:86:PRO:O	1:A:89:GLY:N	2.53	0.41
1:B:201:GLU:O	1:B:204:ARG:HB2	2.20	0.41
1:B:262:LEU:CD1	1:B:262:LEU:N	2.83	0.41
1:A:252:GLY:C	1:A:253:SER:HG	2.23	0.41
1:A:65:GLU:HB2	1:A:302:PHE:HE1	1.84	0.41
1:A:39:PHE:N	1:A:39:PHE:CD1	2.88	0.41
1:A:59:LYS:HE3	1:A:63:GLU:OE2	2.20	0.41
1:A:150:GLU:HA	1:B:194:PHE:CE1	2.55	0.41
1:B:27:ASP:HB2	1:B:32:LEU:HD11	2.02	0.41
1:B:317:LYS:HD3	1:B:343:THR:CG2	2.50	0.41
1:A:163:GLU:HB3	1:A:167:ARG:NH2	2.35	0.41
1:A:109:PHE:HB2	1:A:112:LEU:HD22	2.02	0.41
1:A:53:PHE:CE1	1:A:57:THR:HG22	2.55	0.41
1:B:118:LEU:HD13	1:B:122:ILE:CG2	2.50	0.41
1:B:246:LEU:O	1:B:249:VAL:CG2	2.66	0.41
1:B:314:ALA:CB	1:B:344:VAL:HG12	2.49	0.41
1:B:53:PHE:CD2	1:B:58:ARG:NH1	2.89	0.41
1:B:181:VAL:HG21	1:B:230:PHE:CD1	2.55	0.41
1:A:78:ASP:HA	1:A:85:ARG:HD2	2.03	0.41
1:B:343:THR:HA	1:B:346:ILE:HD12	2.03	0.41
1:B:81:PRO:CD	1:B:84:ILE:HD11	2.25	0.41
1:A:190:GLU:OE2	1:B:144:ARG:HB2	2.21	0.41
1:A:196:ARG:NH2	1:A:213:HIS:CB	2.84	0.41
1:A:239:PHE:O	1:A:243:LEU:HD22	2.20	0.41
1:A:324:PRO:HG3	1:A:336:PHE:CD1	2.55	0.40
1:A:76:LYS:HG2	1:A:76:LYS:O	2.19	0.40
1:B:270:GLU:HG3	1:B:271:PRO:O	2.21	0.40
1:A:138:ILE:HA	1:A:154:THR:O	2.21	0.40
1:B:114:ARG:HG3	1:B:115:LEU:HD13	2.03	0.40
1:B:107:LYS:HE2	1:B:127:ASP:OD2	2.21	0.40
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.92	0.40
1:B:22:VAL:O	1:B:26:LEU:HD13	2.21	0.40
1:A:1:MET:HG3	1:A:302:PHE:CE2	2.57	0.40
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.77	0.40

All (1) 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)
2:A:352:HOH:O	2:B:364:HOH:O[2_856]	1.71	0.49

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	344/346 (99%)	319 (93%)	21 (6%)	4 (1%)	13	10
1	B	344/346 (99%)	327 (95%)	16 (5%)	1 (0%)	41	46
All	All	688/692 (99%)	646 (94%)	37 (5%)	5 (1%)	22	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	SER
1	A	305	VAL
1	B	188	VAL
1	A	84	ILE
1	A	188	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/267 (100%)	216 (81%)	51 (19%)	1	1
1	B	267/267 (100%)	223 (84%)	44 (16%)	2	1
All	All	534/534 (100%)	439 (82%)	95 (18%)	2	1

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	38	VAL
1	A	51	GLU
1	A	53	PHE
1	A	55	GLU
1	A	63	GLU
1	A	65	GLU
1	A	68	LEU
1	A	78	ASP
1	A	83	LYS
1	A	84	ILE
1	A	90	LEU
1	A	104	ARG
1	A	114	ARG
1	A	118	LEU
1	A	120	GLU
1	A	122	ILE
1	A	124	ARG
1	A	130	ILE
1	A	148	GLU
1	A	150	GLU
1	A	156	ARG
1	A	165	VAL
1	A	172	LEU
1	A	225	ARG
1	A	229	ARG
1	A	243	LEU
1	A	244	SER
1	A	250	LEU
1	A	253	SER
1	A	254	LEU
1	A	259	SER
1	A	262	LEU
1	A	264	ARG
1	A	266	THR
1	A	270	GLU
1	A	275	SER
1	A	284	ILE
1	A	286	ASN
1	A	293	SER
1	A	298	LEU
1	A	299	GLU

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Mol	Chain	Res	Type
1	A	304	LEU
1	A	309	ARG
1	A	310	LYS
1	A	315	VAL
1	A	320	LEU
1	A	327	LEU
1	A	344	VAL
1	A	346	ILE
1	B	11	ILE
1	B	23	LEU
1	B	30	GLU
1	B	38	VAL
1	B	55	GLU
1	B	58	ARG
1	B	59	LYS
1	B	63	GLU
1	B	71	SER
1	B	80	LEU
1	B	83	LYS
1	B	87	GLU
1	B	90	LEU
1	B	91	LEU
1	B	92	SER
1	B	93	LEU
1	B	94	ARG
1	B	95	LYS
1	B	104	ARG
1	B	115	LEU
1	B	120	GLU
1	B	130	ILE
1	B	144	ARG
1	B	148	GLU
1	B	157	TYR
1	B	164	ARG
1	B	172	LEU
1	B	185	LYS
1	B	200	GLU
1	B	201	GLU
1	B	219	MET
1	B	241	ASP
1	B	250	LEU
1	B	259	SER

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Mol	Chain	Res	Type
1	B	262	LEU
1	B	264	ARG
1	B	270	GLU
1	B	284	ILE
1	B	286	ASN
1	B	305	VAL
1	B	307	LEU
1	B	309	ARG
1	B	310	LYS
1	B	341	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	286	ASN
1	B	286	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 carbohydrates 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 [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	346/346 (100%)	-0.50	4 (1%) 79 77	18, 39, 64, 93	0
1	B	346/346 (100%)	-0.70	0 100 100	14, 36, 56, 69	0
All	All	692/692 (100%)	-0.60	4 (0%) 89 88	14, 38, 59, 93	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	GLY	3.1
1	A	345	GLY	3.0
1	A	48	ALA	2.5
1	A	254	LEU	2.2

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 carbohydrates 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.