



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 09:51 PM EDT

PDB ID : 3KRN
Title : Crystal Structure of *C. elegans* cell-death-related nuclease 5(CRN-5)
Authors : Yang, C.-C.; Wang, Y.-T.; Hsiao, Y.-Y.; Doudeva, L.G.; Chow, S.Y.; Yuan, H.S.
Deposited on : 2009-11-19
Resolution : 3.92 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

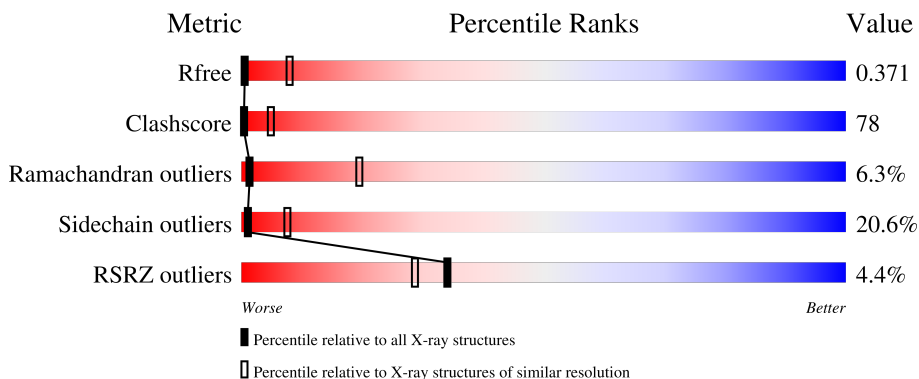
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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	222	
1	B	222	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2575 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 C14A4.5, confirmed by transcript evidence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	183	1374	864	235	261	14	0	0	0
1	B	160	1201	758	205	225	13	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	LEU	-	expression tag	UNP Q17952
A	216	GLU	-	expression tag	UNP Q17952
A	217	HIS	-	expression tag	UNP Q17952
A	218	HIS	-	expression tag	UNP Q17952
A	219	HIS	-	expression tag	UNP Q17952
A	220	HIS	-	expression tag	UNP Q17952
A	221	HIS	-	expression tag	UNP Q17952
A	222	HIS	-	expression tag	UNP Q17952
B	215	LEU	-	expression tag	UNP Q17952
B	216	GLU	-	expression tag	UNP Q17952
B	217	HIS	-	expression tag	UNP Q17952
B	218	HIS	-	expression tag	UNP Q17952
B	219	HIS	-	expression tag	UNP Q17952
B	220	HIS	-	expression tag	UNP Q17952
B	221	HIS	-	expression tag	UNP Q17952
B	222	HIS	-	expression tag	UNP Q17952

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.95Å 44.84Å 65.51Å 90.00° 100.65° 90.00°	Depositor
Resolution (Å)	26.50 – 3.92 36.79 – 3.92	Depositor EDS
% Data completeness (in resolution range)	97.2 (26.50-3.92) 85.1 (36.79-3.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.39 (at 3.87Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.306 , 0.356 0.302 , 0.371	Depositor DCC
R_{free} test set	228 reflections (7.06%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtrriage
Anisotropy	0.360	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 99.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2575	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.78% 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	0.29	0/1394	0.50	0/1878
1	B	0.28	0/1219	0.55	0/1642
All	All	0.28	0/2613	0.52	0/3520

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	1374	0	1341	209	0
1	B	1201	0	1176	195	0
All	All	2575	0	2517	397	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 78.

All (397) 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:83:LEU:HD11	1:A:121:MET:CG	1.34	1.52
1:A:83:LEU:CD1	1:A:121:MET:HG3	1.73	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:CD1	1:A:121:MET:CG	2.22	1.16
1:A:83:LEU:HD12	1:A:121:MET:HE2	1.29	1.14
1:A:128:CYS:HB2	1:A:129:GLY:CA	1.78	1.13
1:A:128:CYS:CB	1:A:129:GLY:HA2	1.78	1.12
1:A:83:LEU:HD11	1:A:121:MET:HG2	1.15	1.10
1:B:19:ASP:HB3	1:B:119:ASN:HD21	1.09	1.08
1:A:83:LEU:HD11	1:A:121:MET:HG3	1.24	1.06
1:A:83:LEU:CD1	1:A:121:MET:CE	2.36	1.03
1:A:189:LEU:H	1:A:189:LEU:HD22	1.20	1.00
1:A:83:LEU:HD12	1:A:121:MET:CE	1.90	1.00
1:B:207:ARG:O	1:B:211:VAL:HG23	1.65	0.96
1:A:82:ASN:N	1:A:83:LEU:HA	1.81	0.95
1:A:82:ASN:ND2	1:A:89:THR:HB	1.80	0.95
1:A:81:ILE:HG12	1:A:81:ILE:O	1.63	0.94
1:B:77:LEU:HD13	1:B:78:SER:N	1.85	0.92
1:A:82:ASN:HD22	1:A:89:THR:HB	1.31	0.91
1:B:205:MET:SD	1:B:209:LEU:HD11	2.12	0.89
1:A:82:ASN:HD22	1:A:89:THR:CB	1.87	0.88
1:A:83:LEU:CD1	1:A:121:MET:HE2	2.00	0.88
1:A:30:CYS:HB3	1:A:99:GLN:HB3	1.57	0.87
1:B:205:MET:SD	1:B:209:LEU:CD1	2.63	0.87
1:A:183:LEU:HG	1:B:180:PHE:HE2	1.40	0.85
1:B:131:LEU:HB2	1:B:156:LEU:HD12	1.60	0.84
1:B:128:CYS:CB	1:B:129:GLY:HA2	2.09	0.83
1:B:104:MET:HG2	1:B:154:ARG:HH22	1.42	0.83
1:B:19:ASP:HB3	1:B:119:ASN:ND2	1.93	0.83
1:A:183:LEU:HG	1:B:180:PHE:CE2	2.13	0.82
1:A:83:LEU:HD13	1:A:121:MET:HG3	1.62	0.82
1:A:178:TRP:HB3	1:A:182:GLN:HB2	1.60	0.82
1:A:144:THR:HG22	1:A:145:ALA:H	1.45	0.80
1:A:132:ILE:HG13	1:A:139:LEU:HD11	1.66	0.77
1:A:81:ILE:O	1:A:81:ILE:CG1	2.30	0.77
1:A:159:VAL:HB	1:A:169:VAL:HA	1.66	0.77
1:B:166:HIS:HB2	1:B:167:PRO:HD3	1.66	0.77
1:A:189:LEU:HD22	1:A:189:LEU:N	1.98	0.76
1:A:191:GLN:HB3	1:A:192:PRO:HD3	1.68	0.76
1:B:9:ARG:HH11	1:B:9:ARG:CG	1.99	0.76
1:B:79:ASN:HB3	1:B:125:THR:HG22	1.67	0.75
1:B:132:ILE:HG23	1:B:155:VAL:HG13	1.67	0.75
1:B:154:ARG:HD3	1:B:156:LEU:HD11	1.68	0.75
1:A:168:GLU:OE2	1:B:177:HIS:HB3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HD11	1:A:139:LEU:HD21	1.70	0.74
1:B:135:VAL:HG22	1:B:150:ALA:HA	1.70	0.74
1:B:144:THR:HB	1:B:146:LYS:HG2	1.67	0.74
1:A:208:LYS:HA	1:A:211:VAL:HG22	1.67	0.74
1:A:106:ALA:H	1:A:131:LEU:HD23	1.52	0.74
1:A:83:LEU:HD11	1:A:121:MET:SD	2.28	0.73
1:A:189:LEU:O	1:A:192:PRO:HD2	1.87	0.73
1:B:77:LEU:HD13	1:B:77:LEU:C	2.08	0.73
1:B:4:ARG:HE	1:B:4:ARG:N	1.85	0.73
1:A:58:ARG:HA	1:A:59:ALA:HB2	1.70	0.72
1:B:159:VAL:HG12	1:B:169:VAL:HG13	1.71	0.72
1:B:29:THR:HG22	1:B:101:ASP:H	1.53	0.72
1:B:5:LEU:HD13	1:B:5:LEU:H	1.53	0.72
1:A:37:GLY:O	1:A:91:ILE:HD11	1.90	0.71
1:B:103:SER:HA	1:B:143:PRO:HG2	1.73	0.71
1:A:70:ASN:O	1:A:73:ILE:HG23	1.91	0.70
1:A:83:LEU:CD1	1:A:121:MET:HE3	2.18	0.70
1:A:126:VAL:HG23	1:A:161:LYS:HE2	1.73	0.70
1:B:6:ARG:HB2	1:B:142:ASP:CG	2.12	0.70
1:B:9:ARG:HH11	1:B:9:ARG:HG3	1.57	0.70
1:A:199:ASP:O	1:A:203:THR:HG23	1.91	0.70
1:B:31:ILE:HB	1:B:97:GLY:HA2	1.72	0.70
1:A:128:CYS:HB2	1:A:129:GLY:HA2	0.85	0.69
1:A:23:CYS:HB2	1:A:32:TRP:HA	1.74	0.68
1:B:4:ARG:HE	1:B:4:ARG:H	1.40	0.68
1:A:83:LEU:CD1	1:A:121:MET:HG2	2.08	0.68
1:B:147:GLN:O	1:B:150:ALA:HB2	1.93	0.68
1:B:166:HIS:CB	1:B:167:PRO:HD3	2.23	0.68
1:B:204:VAL:HA	1:B:207:ARG:HH21	1.58	0.68
1:A:188:SER:O	1:A:192:PRO:HD3	1.94	0.68
1:A:80:ALA:HB1	1:A:83:LEU:C	2.15	0.67
1:B:207:ARG:O	1:B:211:VAL:CG2	2.42	0.67
1:B:140:ILE:HD11	1:B:142:ASP:O	1.93	0.67
1:B:24:PHE:CZ	1:B:26:GLN:HG2	2.29	0.67
1:A:69:LEU:HD13	1:A:69:LEU:O	1.95	0.67
1:A:193:SER:O	1:A:197:ILE:HG22	1.95	0.67
1:A:172:MET:HG2	1:B:174:ALA:HB3	1.78	0.66
1:B:188:SER:O	1:B:189:LEU:HG	1.96	0.66
1:A:31:ILE:HD11	1:A:111:GLY:HA3	1.78	0.66
1:B:157:PHE:HZ	1:B:186:ALA:HB1	1.61	0.66
1:A:14:PHE:CZ	1:A:23:CYS:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HD11	1:A:143:PRO:HA	1.77	0.65
1:A:79:ASN:HA	1:A:80:ALA:HB2	1.77	0.65
1:B:31:ILE:HA	1:B:98:ILE:HG23	1.78	0.65
1:B:33:ALA:HB2	1:B:95:VAL:HG13	1.77	0.65
1:B:156:LEU:H	1:B:156:LEU:HD22	1.61	0.65
1:B:178:TRP:HE3	1:B:182:GLN:HG3	1.62	0.65
1:B:198:PHE:O	1:B:201:TYR:HB2	1.97	0.65
1:B:134:ARG:HA	1:B:139:LEU:HD23	1.79	0.64
1:A:96:HIS:NE2	1:A:98:ILE:HG23	2.11	0.64
1:A:4:ARG:HA	1:A:141:ILE:HG13	1.79	0.64
1:A:14:PHE:CE2	1:A:23:CYS:HB3	2.33	0.64
1:A:82:ASN:N	1:A:83:LEU:CA	2.59	0.64
1:B:81:ILE:HG22	1:B:82:ASN:HB3	1.80	0.64
1:A:103:SER:HA	1:A:131:LEU:HD21	1.80	0.63
1:A:9:ARG:HB3	1:A:25:SER:HB3	1.81	0.63
1:A:189:LEU:H	1:A:189:LEU:CD2	2.00	0.63
1:B:79:ASN:C	1:B:79:ASN:HD22	2.02	0.63
1:A:89:THR:O	1:A:91:ILE:HD13	1.98	0.63
1:A:161:LYS:CD	1:A:161:LYS:H	2.11	0.63
1:B:128:CYS:SG	1:B:194:ALA:HB1	2.39	0.63
1:A:80:ALA:CB	1:A:83:LEU:C	2.67	0.62
1:B:166:HIS:HB2	1:B:167:PRO:CD	2.30	0.62
1:A:24:PHE:HB2	1:A:111:GLY:HA3	1.80	0.62
1:A:178:TRP:N	1:A:178:TRP:CD1	2.67	0.61
1:A:185:ALA:O	1:A:189:LEU:CD2	2.48	0.61
1:A:55:ILE:O	1:A:55:ILE:HG12	1.99	0.61
1:B:14:PHE:H	1:B:15:LEU:HD12	1.66	0.61
1:B:114:PHE:CZ	1:B:204:VAL:HG21	2.36	0.61
1:B:191:GLN:HG3	1:B:192:PRO:HD3	1.83	0.61
1:A:6:ARG:HD2	1:A:26:GLN:O	2.00	0.61
1:B:6:ARG:HG2	1:B:27:GLY:HA3	1.81	0.61
1:B:21:SER:O	1:B:22:ALA:HB2	2.01	0.60
1:B:123:PHE:O	1:B:126:VAL:HG13	2.01	0.60
1:A:11:GLU:O	1:A:12:LEU:HD23	2.01	0.60
1:A:188:SER:OG	1:A:189:LEU:HD22	2.02	0.60
1:A:131:LEU:HD12	1:A:131:LEU:O	2.02	0.60
1:A:189:LEU:O	1:A:191:GLN:N	2.35	0.59
1:A:61:CYS:SG	1:A:100:ASP:HB2	2.42	0.59
1:A:180:PHE:HE1	1:B:180:PHE:O	1.85	0.58
1:B:103:SER:HB3	1:B:106:ALA:HB3	1.86	0.58
1:A:57:TYR:HB3	1:A:58:ARG:CZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD11	1:B:205:MET:HG2	1.84	0.58
1:B:178:TRP:CE3	1:B:182:GLN:HG3	2.38	0.58
1:A:126:VAL:HG23	1:A:161:LYS:CE	2.33	0.58
1:B:123:PHE:CZ	1:B:126:VAL:HG11	2.39	0.58
1:B:128:CYS:HB3	1:B:129:GLY:HA2	1.84	0.58
1:B:164:ASP:HA	1:B:166:HIS:CE1	2.39	0.58
1:B:157:PHE:CZ	1:B:186:ALA:HB1	2.39	0.58
1:B:73:ILE:HD12	1:B:74:HIS:ND1	2.19	0.57
1:A:179:ASP:CG	1:A:180:PHE:H	2.07	0.57
1:B:6:ARG:HB2	1:B:142:ASP:OD1	2.03	0.57
1:A:189:LEU:C	1:A:191:GLN:H	2.07	0.57
1:B:128:CYS:HB2	1:B:129:GLY:HA2	1.85	0.57
1:B:103:SER:CB	1:B:106:ALA:HB3	2.35	0.57
1:A:144:THR:HG22	1:A:145:ALA:N	2.16	0.57
1:B:157:PHE:HB2	1:B:159:VAL:HG13	1.86	0.57
1:A:125:THR:HA	1:A:160:CYS:SG	2.45	0.57
1:B:24:PHE:CE2	1:B:110:ASN:HB2	2.40	0.57
1:B:73:ILE:HD12	1:B:74:HIS:H	1.69	0.57
1:A:25:SER:HA	1:A:30:CYS:HA	1.87	0.56
1:A:178:TRP:HE3	1:A:182:GLN:O	1.88	0.56
1:B:12:LEU:CD1	1:B:13:SER:H	2.18	0.56
1:B:156:LEU:HD22	1:B:156:LEU:N	2.20	0.56
1:A:195:SER:HA	1:A:198:PHE:CD1	2.41	0.56
1:B:189:LEU:C	1:B:192:PRO:HD2	2.26	0.56
1:B:12:LEU:CB	1:B:208:LYS:HE2	2.36	0.56
1:A:181:ILE:HG13	1:A:182:GLN:N	2.20	0.56
1:B:132:ILE:HG13	1:B:139:LEU:HD11	1.88	0.56
1:A:81:ILE:C	1:A:83:LEU:HA	2.25	0.56
1:A:197:ILE:CG1	1:A:201:TYR:HE1	2.19	0.56
1:A:57:TYR:HB2	1:A:69:LEU:HD12	1.88	0.55
1:A:166:HIS:ND1	1:A:166:HIS:N	2.54	0.55
1:A:204:VAL:O	1:A:207:ARG:HB2	2.06	0.55
1:B:191:GLN:O	1:B:194:ALA:HB3	2.05	0.55
1:B:114:PHE:HE2	1:B:204:VAL:HG11	1.72	0.55
1:A:139:LEU:HD13	1:A:140:ILE:N	2.22	0.55
1:B:104:MET:HG2	1:B:154:ARG:NH2	2.16	0.55
1:B:155:VAL:C	1:B:156:LEU:HD13	2.27	0.55
1:B:157:PHE:HZ	1:B:186:ALA:CB	2.20	0.55
1:A:139:LEU:HD22	1:A:140:ILE:H	1.71	0.54
1:B:124:GLU:HG3	1:B:125:THR:HG23	1.87	0.54
1:A:24:PHE:HB2	1:A:111:GLY:CA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:HB	1:A:107:VAL:HG21	1.88	0.54
1:B:202:LYS:O	1:B:206:LYS:HB2	2.07	0.54
1:B:12:LEU:HB2	1:B:208:LYS:HE2	1.89	0.54
1:A:109:ILE:HG23	1:A:129:GLY:H	1.73	0.54
1:B:29:THR:OG1	1:B:107:VAL:HG21	2.07	0.54
1:B:77:LEU:C	1:B:77:LEU:CD1	2.76	0.54
1:A:132:ILE:CG1	1:A:139:LEU:HD11	2.37	0.54
1:A:187:TRP:HB2	1:B:180:PHE:CZ	2.42	0.54
1:A:96:HIS:CE1	1:A:98:ILE:HG23	2.43	0.54
1:A:14:PHE:O	1:A:15:LEU:C	2.45	0.54
1:B:19:ASP:CB	1:B:119:ASN:HD21	2.00	0.54
1:B:150:ALA:O	1:B:152:THR:N	2.41	0.54
1:A:23:CYS:SG	1:A:31:ILE:O	2.66	0.54
1:A:74:HIS:CG	1:A:109:ILE:HD12	2.43	0.54
1:A:181:ILE:HG13	1:A:182:GLN:HG2	1.90	0.54
1:B:127:PHE:CD2	1:B:127:PHE:N	2.76	0.53
1:B:25:SER:HA	1:B:30:CYS:HA	1.90	0.53
1:B:9:ARG:HH22	1:B:11:GLU:HG2	1.73	0.53
1:B:96:HIS:CD2	1:B:98:ILE:HG22	2.44	0.53
1:A:200:PHE:O	1:A:204:VAL:HG23	2.09	0.53
1:A:180:PHE:HZ	1:B:181:ILE:HA	1.73	0.53
1:A:4:ARG:O	1:A:142:ASP:HB3	2.09	0.53
1:A:132:ILE:HB	1:A:141:ILE:HG22	1.91	0.53
1:A:96:HIS:CG	1:A:97:GLY:N	2.77	0.53
1:A:194:ALA:O	1:A:197:ILE:HG23	2.09	0.53
1:A:161:LYS:HZ2	1:A:161:LYS:N	2.06	0.53
1:B:131:LEU:HD13	1:B:156:LEU:HD12	1.91	0.52
1:A:148:GLU:CD	1:A:154:ARG:HH12	2.12	0.52
1:A:159:VAL:HG21	1:A:167:PRO:HB2	1.92	0.52
1:A:36:SER:O	1:A:91:ILE:HG13	2.09	0.52
1:A:68:VAL:HG22	1:A:68:VAL:O	2.08	0.52
1:A:132:ILE:HA	1:A:141:ILE:O	2.08	0.52
1:B:80:ALA:HB1	1:B:81:ILE:HA	1.92	0.52
1:A:123:PHE:C	1:A:123:PHE:CD2	2.83	0.52
1:B:73:ILE:O	1:B:76:THR:HG22	2.10	0.52
1:B:9:ARG:CG	1:B:9:ARG:NH1	2.66	0.51
1:B:114:PHE:CE2	1:B:204:VAL:HG21	2.46	0.51
1:B:139:LEU:HD22	1:B:140:ILE:N	2.25	0.51
1:A:82:ASN:ND2	1:A:89:THR:CB	2.56	0.51
1:A:116:LEU:HD23	1:A:116:LEU:H	1.75	0.51
1:A:117:LEU:HD13	1:A:117:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:N	1:A:178:TRP:CZ2	2.79	0.51
1:B:12:LEU:HD13	1:B:13:SER:H	1.75	0.51
1:B:132:ILE:HG12	1:B:139:LEU:HD21	1.92	0.51
1:B:128:CYS:CB	1:B:129:GLY:CA	2.86	0.51
1:A:31:ILE:HG23	1:A:107:VAL:HG12	1.92	0.51
1:A:67:ASN:ND2	1:A:70:ASN:H	2.09	0.50
1:B:167:PRO:HD2	1:B:168:GLU:H	1.75	0.50
1:A:82:ASN:OD1	1:A:82:ASN:O	2.30	0.50
1:A:189:LEU:C	1:A:191:GLN:N	2.65	0.50
1:B:201:TYR:O	1:B:204:VAL:HG23	2.12	0.50
1:B:157:PHE:HA	1:B:172:MET:HA	1.94	0.50
1:A:11:GLU:HB2	1:A:14:PHE:CZ	2.46	0.50
1:A:23:CYS:SG	1:A:23:CYS:O	2.70	0.50
1:A:74:HIS:CD2	1:A:75:SER:N	2.80	0.50
1:B:123:PHE:CE1	1:B:126:VAL:HG11	2.47	0.50
1:B:182:GLN:HA	1:B:182:GLN:HE21	1.75	0.50
1:A:22:ALA:HB3	1:A:115:ALA:HA	1.93	0.50
1:A:113:CYS:SG	1:A:126:VAL:HG12	2.52	0.49
1:B:32:TRP:CE2	1:B:96:HIS:CD2	2.99	0.49
1:B:77:LEU:HD13	1:B:78:SER:CA	2.42	0.49
1:A:24:PHE:HE2	1:A:26:GLN:CG	2.25	0.49
1:A:143:PRO:HB2	1:A:148:GLU:HB2	1.94	0.49
1:A:79:ASN:N	1:A:80:ALA:HA	2.26	0.49
1:B:148:GLU:C	1:B:150:ALA:H	2.14	0.49
1:A:114:PHE:HA	1:A:117:LEU:HB2	1.95	0.49
1:A:161:LYS:H	1:A:161:LYS:HZ2	1.60	0.49
1:A:195:SER:HA	1:A:198:PHE:HD1	1.77	0.48
1:B:205:MET:CG	1:B:209:LEU:HD11	2.42	0.48
1:A:128:CYS:SG	1:A:198:PHE:CE2	3.07	0.48
1:A:154:ARG:N	1:A:178:TRP:CH2	2.81	0.48
1:B:156:LEU:N	1:B:156:LEU:HD13	2.28	0.48
1:A:39:GLY:HA3	1:A:90:THR:O	2.12	0.48
1:B:30:CYS:O	1:B:98:ILE:HG12	2.13	0.48
1:A:26:GLN:NE2	1:A:110:ASN:HD22	2.12	0.48
1:A:55:ILE:O	1:A:55:ILE:CG1	2.61	0.48
1:A:58:ARG:HB3	1:A:71:ASN:HD21	1.79	0.48
1:A:106:ALA:H	1:A:131:LEU:CD2	2.23	0.48
1:B:113:CYS:SG	1:B:201:TYR:HE1	2.36	0.48
1:B:191:GLN:HA	1:B:194:ALA:HB3	1.96	0.48
1:A:119:ASN:ND2	1:A:121:MET:SD	2.87	0.48
1:A:197:ILE:HG12	1:A:201:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ALA:HB2	1:B:83:LEU:C	2.35	0.47
1:B:128:CYS:HB2	1:B:159:VAL:HG23	1.96	0.47
1:B:73:ILE:O	1:B:76:THR:N	2.48	0.47
1:B:191:GLN:N	1:B:192:PRO:CD	2.77	0.47
1:A:71:ASN:O	1:A:74:HIS:CG	2.67	0.47
1:A:126:VAL:HG23	1:A:161:LYS:HZ3	1.79	0.47
1:A:151:SER:O	1:A:152:THR:HG23	2.15	0.47
1:B:200:PHE:O	1:B:201:TYR:C	2.53	0.47
1:A:159:VAL:HG23	1:A:167:PRO:O	2.14	0.47
1:B:29:THR:CG2	1:B:101:ASP:H	2.26	0.47
1:A:157:PHE:HE2	1:A:186:ALA:HB1	1.80	0.47
1:B:81:ILE:HD12	1:B:81:ILE:O	2.15	0.47
1:B:169:VAL:HG12	1:B:170:CYS:N	2.29	0.47
1:A:28:ALA:O	1:A:99:GLN:HG3	2.15	0.47
1:A:58:ARG:N	1:A:59:ALA:HA	2.30	0.47
1:A:159:VAL:HG23	1:A:168:GLU:O	2.15	0.47
1:B:151:SER:C	1:B:152:THR:HG22	2.35	0.47
1:B:134:ARG:HB3	1:B:153:GLY:H	1.80	0.47
1:B:125:THR:O	1:B:127:PHE:HD2	1.98	0.47
1:B:128:CYS:HB3	1:B:129:GLY:CA	2.45	0.47
1:B:194:ALA:O	1:B:197:ILE:HG23	2.14	0.47
1:B:4:ARG:N	1:B:4:ARG:NE	2.59	0.46
1:A:155:VAL:HG13	1:A:178:TRP:CH2	2.50	0.46
1:B:101:ASP:O	1:B:144:THR:HA	2.15	0.46
1:A:161:LYS:HA	1:A:167:PRO:HA	1.97	0.46
1:B:21:SER:O	1:B:22:ALA:CB	2.63	0.46
1:B:106:ALA:O	1:B:110:ASN:CG	2.54	0.46
1:B:131:LEU:C	1:B:131:LEU:HD12	2.36	0.46
1:B:209:LEU:N	1:B:209:LEU:HD12	2.30	0.46
1:A:20:GLY:HA2	1:A:118:ASP:CG	2.35	0.46
1:A:34:SER:HB3	1:A:94:THR:OG1	2.15	0.46
1:A:132:ILE:O	1:A:155:VAL:HG23	2.16	0.46
1:B:74:HIS:ND1	1:B:74:HIS:N	2.63	0.46
1:A:67:ASN:HD22	1:A:70:ASN:H	1.62	0.45
1:A:81:ILE:C	1:A:83:LEU:CA	2.84	0.45
1:B:12:LEU:HG	1:B:208:LYS:HG3	1.97	0.45
1:B:208:LYS:HA	1:B:208:LYS:HD3	1.70	0.45
1:B:182:GLN:HA	1:B:182:GLN:NE2	2.32	0.45
1:A:83:LEU:CD1	1:A:121:MET:SD	2.95	0.45
1:A:140:ILE:HD11	1:A:143:PRO:CA	2.44	0.45
1:B:9:ARG:O	1:B:26:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:SER:HB2	1:B:21:SER:HB2	1.97	0.45
1:A:106:ALA:HB2	1:A:131:LEU:HD23	1.97	0.45
1:A:106:ALA:N	1:A:131:LEU:HD23	2.26	0.45
1:B:8:MET:HA	1:B:26:GLN:HB2	1.99	0.45
1:A:188:SER:O	1:A:189:LEU:C	2.54	0.45
1:B:118:ASP:HB2	1:B:205:MET:CE	2.46	0.45
1:B:131:LEU:HA	1:B:156:LEU:HA	1.99	0.45
1:A:66:PHE:CG	1:A:67:ASN:N	2.85	0.45
1:A:106:ALA:CB	1:A:131:LEU:HD23	2.46	0.45
1:A:179:ASP:O	1:A:183:LEU:HB2	2.16	0.45
1:A:194:ALA:HA	1:A:197:ILE:CG2	2.46	0.45
1:B:125:THR:O	1:B:127:PHE:CD2	2.69	0.45
1:B:205:MET:SD	1:B:209:LEU:HD12	2.53	0.45
1:B:205:MET:HG3	1:B:209:LEU:HD11	1.98	0.45
1:B:4:ARG:HD2	1:B:4:ARG:C	2.36	0.45
1:B:152:THR:HA	1:B:153:GLY:HA3	1.60	0.45
1:A:61:CYS:SG	1:A:62:GLY:N	2.90	0.45
1:A:132:ILE:HG23	1:A:155:VAL:HG23	1.99	0.45
1:B:134:ARG:HD2	1:B:182:GLN:OE1	2.17	0.45
1:A:24:PHE:HE2	1:A:26:GLN:HG2	1.82	0.44
1:A:55:ILE:O	1:A:56:SER:HB2	2.17	0.44
1:B:24:PHE:CE2	1:B:26:GLN:HG2	2.51	0.44
1:B:113:CYS:SG	1:B:201:TYR:CE1	3.11	0.44
1:A:93:VAL:O	1:A:95:VAL:HG23	2.17	0.44
1:A:58:ARG:HB2	1:A:69:LEU:HD11	1.98	0.44
1:A:156:LEU:HD12	1:A:173:ASP:HB3	2.00	0.44
1:A:169:VAL:HG11	1:A:187:TRP:CD1	2.52	0.44
1:B:4:ARG:C	1:B:4:ARG:CD	2.86	0.44
1:B:113:CYS:HG	1:B:201:TYR:HE1	1.62	0.44
1:A:70:ASN:O	1:A:73:ILE:HD12	2.18	0.44
1:A:80:ALA:HB1	1:A:83:LEU:O	2.18	0.44
1:B:150:ALA:C	1:B:151:SER:HG	2.21	0.44
1:B:95:VAL:HG12	1:B:96:HIS:N	2.32	0.44
1:B:14:PHE:H	1:B:15:LEU:CD1	2.31	0.44
1:B:79:ASN:C	1:B:79:ASN:ND2	2.69	0.44
1:A:83:LEU:HD13	1:A:121:MET:HE3	1.97	0.43
1:A:116:LEU:H	1:A:116:LEU:CD2	2.31	0.43
1:B:105:GLY:O	1:B:109:ILE:N	2.51	0.43
1:B:132:ILE:HD13	1:B:132:ILE:O	2.17	0.43
1:A:7:GLU:O	1:A:27:GLY:N	2.51	0.43
1:B:117:LEU:CD2	1:B:123:PHE:HD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PHE:CE2	1:B:126:VAL:HG11	2.53	0.43
1:A:138:GLU:HB3	1:A:139:LEU:H	1.69	0.43
1:A:126:VAL:HG23	1:A:161:LYS:NZ	2.33	0.43
1:A:160:CYS:O	1:A:167:PRO:O	2.36	0.43
1:B:103:SER:CA	1:B:143:PRO:HG2	2.45	0.43
1:B:131:LEU:HB2	1:B:156:LEU:HB3	2.00	0.43
1:B:133:VAL:HA	1:B:154:ARG:H	1.84	0.43
1:A:69:LEU:C	1:A:69:LEU:HD22	2.39	0.43
1:A:203:THR:O	1:A:207:ARG:HG2	2.19	0.43
1:A:35:CYS:SG	1:A:36:SER:N	2.91	0.43
1:A:109:ILE:CG2	1:A:129:GLY:H	2.31	0.43
1:B:104:MET:CG	1:B:154:ARG:HH22	2.21	0.43
1:B:121:MET:HA	1:B:122:PRO:HD3	1.89	0.43
1:A:6:ARG:NH1	1:A:28:ALA:HB3	2.33	0.43
1:A:91:ILE:HD12	1:A:91:ILE:HA	1.80	0.43
1:A:131:LEU:HA	1:A:156:LEU:HA	2.01	0.42
1:B:4:ARG:O	1:B:141:ILE:HB	2.18	0.42
1:B:152:THR:O	1:B:152:THR:OG1	2.37	0.42
1:B:105:GLY:CA	1:B:109:ILE:HD13	2.49	0.42
1:B:27:GLY:C	1:B:29:THR:H	2.22	0.42
1:B:77:LEU:HD21	1:B:83:LEU:O	2.20	0.42
1:B:147:GLN:O	1:B:150:ALA:CB	2.66	0.42
1:A:36:SER:OG	1:A:91:ILE:HA	2.20	0.42
1:A:67:ASN:HD22	1:A:70:ASN:N	2.16	0.42
1:A:71:ASN:OD1	1:A:72:ILE:N	2.52	0.42
1:A:161:LYS:H	1:A:161:LYS:HD3	1.81	0.42
1:B:177:HIS:O	1:B:178:TRP:CD1	2.73	0.42
1:A:6:ARG:NH2	1:A:143:PRO:O	2.53	0.42
1:A:175:ILE:O	1:A:175:ILE:HG13	2.20	0.42
1:A:93:VAL:O	1:A:93:VAL:HG22	2.19	0.42
1:B:83:LEU:C	1:B:83:LEU:HD23	2.40	0.42
1:B:152:THR:HG23	1:B:178:TRP:NE1	2.35	0.42
1:A:11:GLU:HB2	1:A:14:PHE:CE2	2.55	0.42
1:A:136:LYS:HA	1:A:136:LYS:HD3	1.78	0.42
1:B:200:PHE:CD1	1:B:204:VAL:HG22	2.55	0.42
1:B:128:CYS:SG	1:B:194:ALA:CB	3.07	0.41
1:B:13:SER:HB2	1:B:21:SER:CB	2.50	0.41
1:A:57:TYR:O	1:A:69:LEU:HG	2.21	0.41
1:A:82:ASN:HD22	1:A:89:THR:CG2	2.32	0.41
1:B:117:LEU:HD21	1:B:123:PHE:HD1	1.85	0.41
1:A:7:GLU:HB3	1:A:27:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PHE:O	1:B:203:THR:N	2.54	0.41
1:A:140:ILE:O	1:A:140:ILE:HD13	2.20	0.41
1:B:8:MET:SD	1:B:200:PHE:CD1	3.13	0.41
1:B:35:CYS:HB3	1:B:116:LEU:HD11	2.02	0.41
1:A:11:GLU:O	1:A:14:PHE:HE2	2.03	0.41
1:B:105:GLY:HA2	1:B:109:ILE:HD13	2.01	0.41
1:A:80:ALA:HB3	1:A:83:LEU:C	2.40	0.41
1:B:117:LEU:HD22	1:B:117:LEU:O	2.21	0.41
1:B:131:LEU:CD1	1:B:133:VAL:HG13	2.50	0.41
1:A:26:GLN:O	1:A:28:ALA:N	2.54	0.41
1:A:58:ARG:HD2	1:A:69:LEU:CD1	2.51	0.41
1:A:134:ARG:HB2	1:A:178:TRP:CZ3	2.56	0.41
1:B:119:ASN:C	1:B:121:MET:H	2.23	0.41
1:B:159:VAL:HG12	1:B:169:VAL:HA	2.02	0.41
1:B:188:SER:C	1:B:190:ALA:H	2.23	0.41
1:B:131:LEU:HD11	1:B:133:VAL:HG13	2.02	0.40
1:B:152:THR:CG2	1:B:178:TRP:CD1	3.03	0.40
1:B:191:GLN:HA	1:B:194:ALA:CB	2.50	0.40
1:A:57:TYR:HB2	1:A:69:LEU:CD1	2.49	0.40
1:A:181:ILE:HG13	1:A:182:GLN:H	1.84	0.40
1:B:77:LEU:CD2	1:B:83:LEU:O	2.70	0.40
1:B:105:GLY:O	1:B:106:ALA:C	2.59	0.40
1:B:110:ASN:OD1	1:B:128:CYS:O	2.39	0.40
1:B:128:CYS:SG	1:B:194:ALA:CA	3.09	0.40
1:A:93:VAL:O	1:A:93:VAL:HG13	2.22	0.40
1:B:81:ILE:CG2	1:B:82:ASN:HB3	2.49	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	169/222 (76%)	120 (71%)	38 (22%)	11 (6%)	1	19
1	B	148/222 (67%)	110 (74%)	29 (20%)	9 (6%)	1	20
All	All	317/444 (71%)	230 (73%)	67 (21%)	20 (6%)	1	19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	B	167	PRO
1	A	27	GLY
1	A	67	ASN
1	A	93	VAL
1	A	124	GLU
1	A	126	VAL
1	B	22	ALA
1	B	151	SER
1	A	38	PRO
1	B	119	ASN
1	A	183	LEU
1	A	190	ALA
1	B	143	PRO
1	B	152	THR
1	B	166	HIS
1	A	168	GLU
1	B	201	TYR
1	A	56	SER
1	B	3	GLY

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	149/182 (82%)	120 (80%)	29 (20%)	1	9
1	B	128/182 (70%)	100 (78%)	28 (22%)	1	6
All	All	277/364 (76%)	220 (79%)	57 (21%)	1	7

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	23	CYS
1	A	30	CYS
1	A	55	ILE
1	A	58	ARG
1	A	69	LEU
1	A	73	ILE
1	A	76	THR
1	A	81	ILE
1	A	91	ILE
1	A	119	ASN
1	A	121	MET
1	A	123	PHE
1	A	126	VAL
1	A	128	CYS
1	A	130	VAL
1	A	132	ILE
1	A	140	ILE
1	A	141	ILE
1	A	148	GLU
1	A	152	THR
1	A	159	VAL
1	A	160	CYS
1	A	161	LYS
1	A	166	HIS
1	A	175	ILE
1	A	178	TRP
1	A	180	PHE
1	A	197	ILE
1	B	4	ARG
1	B	5	LEU
1	B	6	ARG
1	B	9	ARG
1	B	12	LEU
1	B	19	ASP
1	B	26	GLN
1	B	73	ILE
1	B	76	THR
1	B	79	ASN
1	B	98	ILE
1	B	101	ASP
1	B	119	ASN

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Mol	Chain	Res	Type
1	B	127	PHE
1	B	128	CYS
1	B	131	LEU
1	B	132	ILE
1	B	140	ILE
1	B	144	THR
1	B	146	LYS
1	B	152	THR
1	B	154	ARG
1	B	156	LEU
1	B	157	PHE
1	B	166	HIS
1	B	191	GLN
1	B	197	ILE
1	B	204	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	26	GLN
1	A	74	HIS
1	A	82	ASN
1	A	119	ASN
1	A	191	GLN
1	B	26	GLN
1	B	79	ASN
1	B	119	ASN
1	B	166	HIS
1	B	191	GLN

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 monosaccharides 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	183/222 (82%)	0.38	11 (6%) 21 17	19, 82, 164, 223	0
1	B	160/222 (72%)	0.38	4 (2%) 57 48	12, 83, 162, 265	0
All	All	343/444 (77%)	0.38	15 (4%) 34 29	12, 82, 162, 265	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	ASN	4.0
1	B	133	VAL	3.7
1	A	125	THR	3.2
1	A	134	ARG	3.0
1	B	25	SER	2.9
1	A	59	ALA	2.8
1	A	34	SER	2.7
1	A	37	GLY	2.6
1	A	67	ASN	2.6
1	A	96	HIS	2.4
1	B	82	ASN	2.3
1	A	65	LYS	2.2
1	B	124	GLU	2.2
1	A	79	ASN	2.1
1	A	68	VAL	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 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.