



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:49 PM UTC

PDB ID : 1UWE / pdb_00001uwe
Title : MOLECULAR MECHANISM OF ENANTIOSELECTIVE PROTON
TRANSFER TO CARBON IN CATALYTIC ANTIBODY 14D9
Authors : Baumann, U.; Reymond, J.L.
Deposited on : 2004-02-05
Resolution : 2.67 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

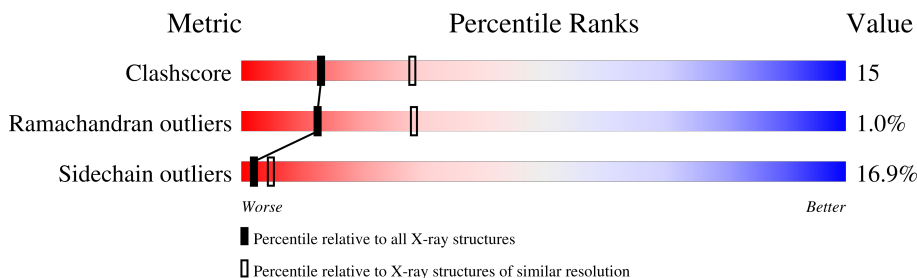
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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))
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	218	62% 29% 8%
1	V	218	70% 26% .
1	Y	218	56% 34% 9%
2	L	213	67% 27% 6%
2	U	213	72% 23% .
2	X	213	70% 25% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9703 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 ANTIBODY 14D9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	0	0
			1612	1023	260	324	5			
1	V	218	Total	C	N	O	S	0	0	0
			1612	1023	260	324	5			
1	Y	218	Total	C	N	O	S	0	0	0
			1612	1023	260	324	5			

- Molecule 2 is a protein called ANTIBODY 14D9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1614	1007	268	333	6			
2	U	213	Total	C	N	O	S	0	0	0
			1614	1007	268	333	6			
2	X	213	Total	C	N	O	S	0	0	0
			1614	1007	268	333	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	O	0	0
			1	1		
3	L	6	Total	O	0	0
			6	6		
3	U	3	Total	O	0	0
			3	3		
3	V	9	Total	O	0	0
			9	9		
3	X	2	Total	O	0	0
			2	2		
3	Y	4	Total	O	0	0
			4	4		

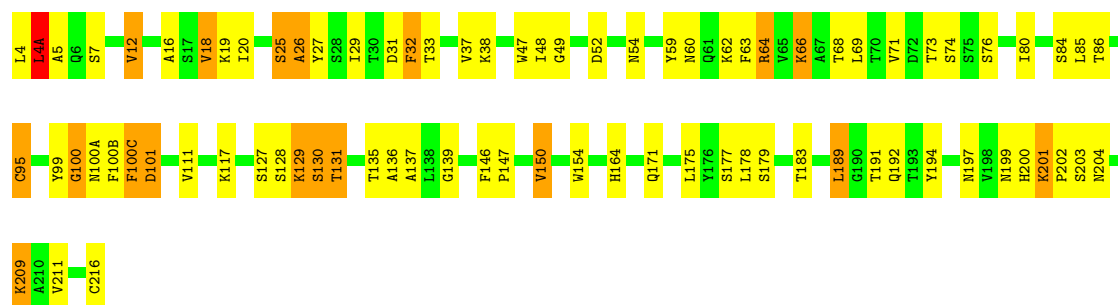
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

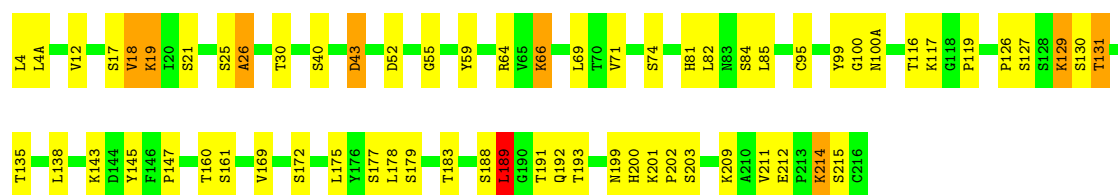
• Molecule 1: ANTIBODY 14D9

Chain H: 



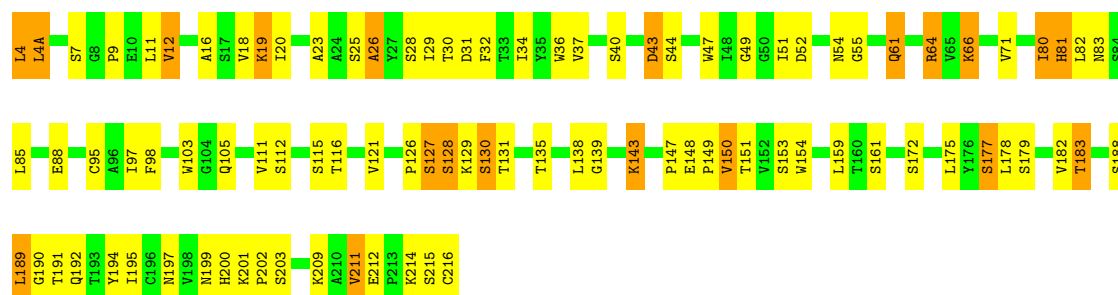
• Molecule 1: ANTIBODY 14D9

Chain V: 



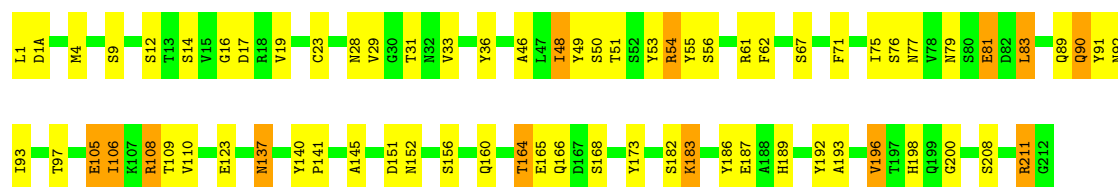
• Molecule 1: ANTIBODY 14D9

Chain Y: 



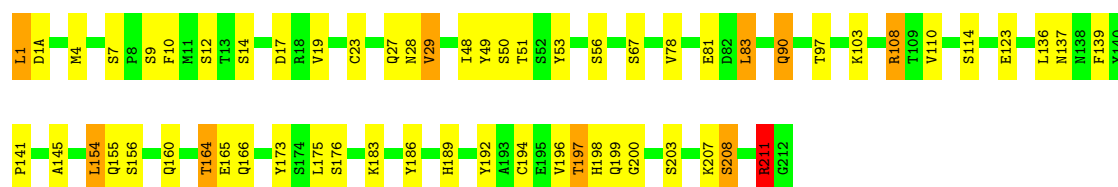
• Molecule 2: ANTIBODY 14D9

Chain L:  67% 27% 6%



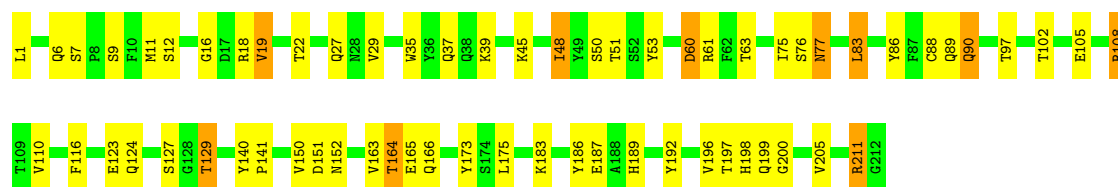
• Molecule 2: ANTIBODY 14D9

Chain U:  72% 23% 5%



• Molecule 2: ANTIBODY 14D9

Chain X:  70% 25% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.10Å 142.79Å 125.46Å 90.00° 104.85° 90.00°	Depositor
Resolution (Å)	20.00 – 2.67	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.67)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.218 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9703	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

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	H	0.73	5/1655 (0.3%)	0.87	3/2263 (0.1%)
1	V	0.44	0/1655	0.81	0/2263
1	Y	0.43	0/1655	0.83	0/2263
2	L	0.59	4/1650 (0.2%)	0.83	0/2250
2	U	0.48	0/1650	0.87	0/2250
2	X	0.39	0/1650	0.82	0/2250
All	All	0.52	9/9915 (0.1%)	0.84	3/13539 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	32	PHE	CG-CD1	13.98	1.68	1.38
1	H	32	PHE	CG-CD2	13.96	1.68	1.38
1	H	32	PHE	CE1-CZ	9.93	1.68	1.38
1	H	32	PHE	CE2-CZ	9.78	1.68	1.38
2	L	55	TYR	CG-CD1	7.07	1.54	1.39
2	L	55	TYR	CE2-CZ	6.65	1.54	1.38
2	L	28	ASN	CG-OD1	6.30	1.35	1.23
1	H	101	ASP	CB-CG	6.23	1.67	1.52
2	L	55	TYR	CG-CD2	5.52	1.50	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	32	PHE	CD1-CG-CD2	6.93	128.99	118.60
1	H	4(A)	LEU	N-CA-C	-5.54	99.00	110.80
1	H	32	PHE	CE1-CZ-CE2	5.52	129.94	120.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1612	0	1554	58	3
1	V	1612	0	1554	38	0
1	Y	1612	0	1552	64	3
2	L	1614	0	1535	56	0
2	U	1614	0	1535	37	0
2	X	1614	0	1535	40	0
3	H	1	0	0	0	0
3	L	6	0	0	0	0
3	U	3	0	0	0	0
3	V	9	0	0	0	0
3	X	2	0	0	1	0
3	Y	4	0	0	1	0
All	All	9703	0	9265	283	3

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 15.

All (283) 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:H:4:LEU:O	1:H:4(A):LEU:C	1.86	1.17
2:U:189:HIS:O	2:U:211:ARG:HD3	1.50	1.11
1:H:100(B):PHE:O	1:H:100(C):PHE:O	1.73	1.07
2:L:108:ARG:HH11	2:L:108:ARG:HG3	0.93	1.05
1:Y:4:LEU:HD23	1:Y:4(A):LEU:H	1.21	1.01
2:L:198:HIS:CD2	2:L:200:GLY:H	1.81	0.98
1:V:12:VAL:HG11	1:V:18:VAL:HG13	1.44	0.97
2:U:108:ARG:HG3	2:U:108:ARG:HH11	1.32	0.94
2:L:198:HIS:HD2	2:L:200:GLY:H	1.14	0.93
2:U:198:HIS:HD2	2:U:200:GLY:H	1.09	0.92
1:Y:19:LYS:HD2	1:Y:81:HIS:NE2	1.83	0.91
1:Y:52:ASP:OD1	1:Y:54:ASN:HB2	1.70	0.91
1:H:100(B):PHE:O	1:H:100(C):PHE:C	2.14	0.89
1:H:4:LEU:O	1:H:4(A):LEU:O	1.89	0.89
2:U:198:HIS:CD2	2:U:200:GLY:H	1.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:192:GLN:NE2	1:Y:194:TYR:OH	2.07	0.86
2:U:29:VAL:HG21	2:U:90:GLN:HG3	1.56	0.86
2:L:29:VAL:HG21	2:L:90:GLN:CG	2.06	0.85
2:L:108:ARG:HG3	2:L:108:ARG:NH1	1.74	0.84
2:X:198:HIS:CD2	2:X:200:GLY:H	1.94	0.84
2:X:164:THR:HG23	2:X:165:GLU:O	1.78	0.84
1:H:12:VAL:HG21	1:H:85:LEU:HD13	1.60	0.83
2:U:29:VAL:CG2	2:U:90:GLN:HG3	2.10	0.81
2:X:108:ARG:HG3	2:X:108:ARG:HH11	1.45	0.81
1:Y:25:SER:O	1:Y:26:ALA:HB3	1.79	0.79
1:V:200:HIS:HD2	1:V:203:SER:OG	1.65	0.79
1:Y:4:LEU:HD23	1:Y:4(A):LEU:N	1.98	0.79
2:X:164:THR:HG21	3:X:2002:HOH:O	1.84	0.77
1:Y:192:GLN:NE2	1:Y:194:TYR:CZ	2.53	0.77
1:H:130:SER:OG	1:H:137:ALA:O	2.02	0.76
2:L:108:ARG:NH1	2:L:109:THR:O	2.20	0.75
1:V:25:SER:O	1:V:26:ALA:HB3	1.87	0.74
1:Y:52:ASP:HB3	1:Y:55:GLY:O	1.87	0.74
2:L:81:GLU:H	2:L:81:GLU:CD	1.95	0.74
1:H:25:SER:O	1:H:26:ALA:HB3	1.87	0.74
1:V:25:SER:O	1:V:26:ALA:CB	2.36	0.73
2:X:108:ARG:HG3	2:X:108:ARG:NH1	2.03	0.73
2:L:29:VAL:HG21	2:L:90:GLN:HG2	1.70	0.73
1:V:127:SER:O	1:V:131:THR:HG22	1.89	0.72
1:V:40:SER:O	1:V:43:ASP:OD1	2.09	0.71
1:H:135:THR:CG2	1:H:183:THR:HG23	2.19	0.71
1:Y:153:SER:OG	1:Y:197:ASN:HB2	1.90	0.71
1:H:101:ASP:OD2	2:L:36:TYR:OH	2.03	0.71
1:Y:40:SER:O	1:Y:43:ASP:OD1	2.08	0.71
2:U:108:ARG:HG3	2:U:108:ARG:NH1	1.93	0.71
2:L:164:THR:CG2	2:L:165:GLU:O	2.39	0.70
1:Y:25:SER:O	1:Y:26:ALA:CB	2.37	0.70
1:H:25:SER:O	1:H:26:ALA:CB	2.39	0.70
1:H:200:HIS:HD2	1:H:203:SER:OG	1.74	0.70
2:L:108:ARG:HH11	2:L:108:ARG:CG	1.85	0.70
1:V:12:VAL:HG11	1:V:18:VAL:CG1	2.21	0.69
2:L:33:VAL:HG21	2:L:71:PHE:CE1	2.27	0.69
2:U:90:GLN:NE2	2:U:97:THR:OG1	2.27	0.68
2:L:164:THR:HG22	2:L:165:GLU:O	1.94	0.67
2:X:198:HIS:HD2	2:X:200:GLY:H	1.42	0.67
1:Y:200:HIS:HD2	1:Y:203:SER:OG	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:12:VAL:HG11	1:Y:18:VAL:HG11	1.76	0.67
2:L:29:VAL:HG21	2:L:90:GLN:HG3	1.76	0.65
2:X:166:GLN:HG3	2:X:173:TYR:CZ	2.31	0.65
1:V:138:LEU:HD13	1:V:211:VAL:HG21	1.78	0.65
1:V:30:THR:HG22	1:V:71:VAL:HG21	1.78	0.65
1:Y:121:VAL:O	1:Y:209:LYS:HE2	1.97	0.65
2:L:83:LEU:HB2	2:L:106:ILE:HD12	1.79	0.64
1:Y:126:PRO:HA	1:Y:130:SER:OG	1.97	0.64
1:H:192:GLN:NE2	1:H:194:TYR:OH	2.31	0.64
2:L:29:VAL:CG2	2:L:90:GLN:CG	2.76	0.64
1:Y:147:PRO:O	1:Y:200:HIS:HE1	1.80	0.63
2:L:14:SER:HB2	2:L:17:ASP:OD2	1.99	0.63
2:U:175:LEU:C	2:U:175:LEU:HD23	2.24	0.63
2:X:151:ASP:O	2:X:152:ASN:HB3	1.98	0.63
2:L:29:VAL:CG2	2:L:90:GLN:HG2	2.29	0.62
2:L:198:HIS:HD2	2:L:200:GLY:N	1.92	0.62
2:U:164:THR:HG23	2:U:165:GLU:O	2.00	0.62
1:H:59:TYR:HE1	1:H:69:LEU:HD13	1.65	0.61
1:V:211:VAL:HG23	1:V:211:VAL:O	2.01	0.61
1:H:4:LEU:O	1:H:5:ALA:N	2.33	0.61
2:X:29:VAL:CG1	2:X:29:VAL:O	2.49	0.61
1:V:178:LEU:C	1:V:178:LEU:HD12	2.26	0.60
2:X:183:LYS:O	2:X:187:GLU:HG2	2.01	0.60
1:H:135:THR:CG2	1:H:183:THR:CG2	2.80	0.60
2:L:89:GLN:HE21	2:L:91:TYR:HD1	1.49	0.60
1:H:203:SER:O	1:H:204:ASN:HB2	1.99	0.60
1:Y:199:ASN:HD22	1:Y:200:HIS:N	2.00	0.59
2:U:4:MET:HE3	2:U:23:CYS:SG	2.42	0.59
2:U:50:SER:O	2:U:51:THR:HB	2.02	0.59
1:H:135:THR:HG23	1:H:183:THR:CG2	2.33	0.58
2:U:208:SER:O	1:V:129:LYS:HE2	2.03	0.58
1:Y:64:ARG:NH1	1:Y:64:ARG:HG2	2.18	0.58
1:H:16:ALA:O	1:H:85:LEU:HD12	2.03	0.58
2:U:198:HIS:HD2	2:U:200:GLY:N	1.90	0.58
1:Y:9:PRO:HD2	1:Y:201:LYS:HD2	1.85	0.58
2:L:61:ARG:HD2	2:L:76:SER:O	2.04	0.58
1:Y:64:ARG:HH11	1:Y:64:ARG:CG	2.16	0.58
1:H:18:VAL:HG22	1:H:85:LEU:HD11	1.86	0.57
1:H:178:LEU:HD12	1:H:178:LEU:C	2.29	0.57
1:H:135:THR:HG23	1:H:183:THR:HG23	1.86	0.56
1:H:147:PRO:O	1:H:200:HIS:HE1	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:66:LYS:O	1:Y:66:LYS:HG3	2.05	0.56
1:Y:201:LYS:N	1:Y:202:PRO:CD	2.68	0.56
2:X:50:SER:O	2:X:51:THR:HB	2.05	0.56
1:V:12:VAL:CG1	1:V:18:VAL:HG13	2.27	0.56
2:U:17:ASP:O	2:U:78:VAL:HG23	2.06	0.56
2:U:108:ARG:HH11	2:U:108:ARG:CG	2.08	0.56
1:Y:20:ILE:HB	1:Y:80:ILE:CG2	2.37	0.55
1:H:32:PHE:CD1	1:H:100(C):PHE:HZ	2.25	0.55
1:Y:61:GLN:HA	1:Y:64:ARG:HG3	1.88	0.55
2:L:49:TYR:CZ	2:L:53:TYR:HB3	2.42	0.55
1:Y:47:TRP:CZ2	1:Y:49:GLY:HA2	2.42	0.55
1:Y:12:VAL:HG11	1:Y:18:VAL:CG1	2.37	0.55
2:U:154:LEU:HD12	2:U:155:GLN:N	2.22	0.55
2:X:37:GLN:OE1	2:X:39:LYS:HE3	2.07	0.54
1:H:60:ASN:HB3	1:H:63:PHE:HD2	1.72	0.54
2:X:16:GLY:HA2	2:X:77:ASN:HD22	1.72	0.54
2:X:29:VAL:O	2:X:29:VAL:HG12	2.06	0.54
2:L:151:ASP:O	2:L:152:ASN:HB2	2.07	0.54
2:X:124:GLN:HG2	2:X:129:THR:O	2.07	0.54
1:Y:127:SER:O	1:Y:129:LYS:N	2.41	0.54
2:L:29:VAL:CG2	2:L:90:GLN:HG3	2.36	0.54
2:L:33:VAL:HG21	2:L:71:PHE:CZ	2.43	0.53
1:V:201:LYS:N	1:V:202:PRO:CD	2.71	0.53
2:U:49:TYR:CE1	1:V:100(A):ASN:HB3	2.44	0.53
1:V:99:TYR:O	1:V:100:GLY:C	2.52	0.53
1:H:4(A):LEU:HD13	1:H:95:CYS:SG	2.49	0.53
1:Y:105:GLN:HB2	3:Y:2001:HOH:O	2.09	0.53
1:H:150:VAL:O	1:H:150:VAL:CG1	2.57	0.52
1:H:171:GLN:NE2	1:H:177:SER:HB2	2.24	0.52
1:H:4(A):LEU:H	1:H:4(A):LEU:HD23	1.75	0.52
2:U:27:GLN:O	2:U:28:ASN:C	2.53	0.52
1:Y:64:ARG:HG2	1:Y:64:ARG:HH11	1.74	0.52
2:L:33:VAL:CG2	2:L:71:PHE:CE1	2.93	0.52
2:X:186:TYR:O	2:X:192:TYR:OH	2.28	0.52
2:X:108:ARG:HH11	2:X:108:ARG:CG	2.19	0.52
1:H:100(A):ASN:O	1:H:100(B):PHE:CD1	2.63	0.52
1:Y:28:SER:HB3	1:Y:31:ASP:OD2	2.10	0.51
1:Y:138:LEU:HD13	1:Y:211:VAL:HG21	1.93	0.51
2:L:189:HIS:O	2:L:211:ARG:HD3	2.10	0.51
1:V:30:THR:HG22	1:V:71:VAL:CG2	2.40	0.51
2:X:1:LEU:HD23	2:X:1:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:52:ASP:OD1	1:Y:54:ASN:CB	2.54	0.51
1:V:188:SER:HB2	1:V:192:GLN:HE22	1.76	0.51
2:X:6:GLN:NE2	2:X:86:TYR:O	2.40	0.51
2:L:81:GLU:CD	2:L:81:GLU:N	2.66	0.51
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.46	0.50
2:U:136:LEU:N	2:U:136:LEU:HD12	2.26	0.50
2:X:150:VAL:HG12	2:X:189:HIS:CD2	2.46	0.50
2:L:89:GLN:HG2	2:L:90:GLN:N	2.27	0.50
1:V:18:VAL:HG22	1:V:85:LEU:HD11	1.92	0.50
2:X:16:GLY:HA2	2:X:77:ASN:ND2	2.27	0.50
1:H:12:VAL:HG21	1:H:85:LEU:CD1	2.35	0.50
1:H:99:TYR:O	1:H:100:GLY:C	2.55	0.50
2:U:49:TYR:CZ	1:V:100(A):ASN:HB3	2.46	0.50
2:L:77:ASN:O	2:L:79:ASN:ND2	2.45	0.50
1:V:147:PRO:O	1:V:200:HIS:HE1	1.94	0.50
1:H:33:THR:OG1	1:H:52:ASP:HB2	2.12	0.50
1:V:43:ASP:OD1	1:V:43:ASP:N	2.44	0.50
1:V:211:VAL:O	1:V:211:VAL:CG2	2.59	0.49
1:Y:148:GLU:HB3	1:Y:149:PRO:HA	1.94	0.49
1:H:59:TYR:CE1	1:H:69:LEU:HD13	2.46	0.49
1:Y:64:ARG:NH1	1:Y:64:ARG:CG	2.75	0.49
1:H:101:ASP:HB3	2:L:46:ALA:CB	2.43	0.49
2:X:150:VAL:HG12	2:X:189:HIS:HD2	1.78	0.48
1:Y:11:LEU:HD23	1:Y:116:THR:HG23	1.94	0.48
1:Y:11:LEU:HD11	1:Y:112:SER:HB3	1.95	0.48
1:Y:199:ASN:HD22	1:Y:200:HIS:H	1.60	0.48
2:L:4:MET:HE3	2:L:23:CYS:SG	2.53	0.48
1:Y:127:SER:O	1:Y:130:SER:N	2.27	0.48
1:H:201:LYS:N	1:H:202:PRO:CD	2.76	0.48
1:Y:127:SER:O	1:Y:131:THR:HG23	2.13	0.48
1:Y:188:SER:O	1:Y:190:GLY:N	2.46	0.48
1:H:192:GLN:CD	1:H:192:GLN:H	2.21	0.48
2:L:164:THR:HG23	2:L:165:GLU:O	2.13	0.48
2:U:160:GLN:NE2	1:V:169:VAL:HG12	2.28	0.48
1:Y:159:LEU:HD21	1:Y:182:VAL:HG21	1.95	0.48
2:L:83:LEU:HD21	2:L:166:GLN:O	2.13	0.48
2:U:175:LEU:HD23	2:U:176:SER:N	2.28	0.48
2:L:186:TYR:HA	2:L:192:TYR:OH	2.14	0.48
2:L:76:SER:O	2:L:77:ASN:C	2.57	0.48
1:Y:135:THR:HG23	1:Y:183:THR:HG23	1.96	0.48
2:L:140:TYR:CG	2:L:141:PRO:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:89:GLN:HG2	2:X:90:GLN:N	2.27	0.47
1:H:200:HIS:HD2	1:H:203:SER:CB	2.27	0.47
2:X:151:ASP:O	2:X:152:ASN:CB	2.62	0.47
1:Y:37:VAL:HG21	1:Y:103:TRP:CH2	2.49	0.47
2:U:1:LEU:HD23	2:U:1:LEU:O	2.15	0.47
1:Y:66:LYS:HB2	1:Y:66:LYS:HE3	1.57	0.47
1:Y:139:GLY:HA2	1:Y:154:TRP:CH2	2.49	0.47
1:Y:143:LYS:HA	1:Y:177:SER:OG	2.14	0.47
1:V:52:ASP:HB3	1:V:55:GLY:O	2.15	0.47
1:H:164:HIS:CD2	2:L:137:ASN:HD21	2.33	0.47
1:H:130:SER:OG	1:H:130:SER:O	2.33	0.47
2:L:50:SER:O	2:L:51:THR:HB	2.15	0.47
1:Y:150:VAL:O	1:Y:150:VAL:CG1	2.61	0.47
1:H:32:PHE:CE1	1:H:100(C):PHE:HZ	2.34	0.46
1:V:82:LEU:HB3	1:V:85:LEU:HD21	1.96	0.46
2:X:150:VAL:CG1	2:X:189:HIS:HD2	2.28	0.46
2:L:61:ARG:HG2	2:L:61:ARG:HH11	1.80	0.46
1:V:12:VAL:HG21	1:V:85:LEU:HD12	1.97	0.46
1:V:19:LYS:NZ	1:V:81:HIS:HB2	2.30	0.46
2:X:164:THR:CG2	2:X:165:GLU:O	2.58	0.46
1:H:64:ARG:NH1	1:H:64:ARG:HG2	2.31	0.46
1:Y:36:TRP:CZ3	1:Y:95:CYS:HB3	2.50	0.46
1:H:32:PHE:CD1	1:H:100(C):PHE:CZ	3.04	0.46
2:L:29:VAL:HG22	2:L:29:VAL:O	2.15	0.46
1:Y:138:LEU:HD12	1:Y:138:LEU:C	2.41	0.45
1:Y:34:ILE:HG13	1:Y:97:ILE:HG22	1.97	0.45
2:U:154:LEU:HD12	2:U:154:LEU:C	2.42	0.45
1:V:119:PRO:HB3	1:V:145:TYR:HB3	1.98	0.45
1:Y:11:LEU:CD2	1:Y:116:THR:HG23	2.46	0.45
2:L:54:ARG:HD3	2:L:62:PHE:O	2.17	0.45
2:U:164:THR:CG2	2:U:165:GLU:O	2.64	0.45
1:Y:127:SER:C	1:Y:129:LYS:N	2.73	0.45
1:Y:12:VAL:HG23	1:Y:16:ALA:HB3	1.98	0.45
1:H:66:LYS:HB2	1:H:66:LYS:HE2	1.41	0.45
2:L:90:GLN:NE2	2:L:97:THR:OG1	2.49	0.45
2:U:139:PHE:HD2	2:U:198:HIS:CE1	2.35	0.45
1:V:126:PRO:HA	1:V:130:SER:OG	2.16	0.44
1:V:214:LYS:HB2	1:V:214:LYS:HE2	1.52	0.44
2:X:12:SER:HA	2:X:105:GLU:O	2.17	0.44
1:H:189:LEU:HD12	1:H:189:LEU:HA	1.80	0.44
2:U:166:GLN:HG3	2:U:173:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:178:LEU:HD12	1:Y:178:LEU:C	2.42	0.44
1:Y:192:GLN:O	1:Y:192:GLN:HG2	2.13	0.44
1:H:146:PHE:HA	1:H:147:PRO:HA	1.77	0.44
2:X:60:ASP:OD1	2:X:60:ASP:N	2.50	0.44
2:L:62:PHE:CD1	2:L:75:ILE:HG12	2.53	0.44
2:U:83:LEU:HD21	2:U:166:GLN:O	2.18	0.44
1:Y:82:LEU:HB3	1:Y:85:LEU:HD21	1.98	0.44
1:H:127:SER:O	1:H:131:THR:CG2	2.66	0.43
1:H:209:LYS:HA	1:H:209:LYS:HD3	1.77	0.43
2:X:19:VAL:HG12	2:X:75:ILE:HB	2.00	0.43
1:Y:150:VAL:HG23	1:Y:200:HIS:HB2	1.99	0.43
2:U:10:PHE:HD1	2:U:103:LYS:HB3	1.83	0.43
2:U:48:ILE:HA	2:U:53:TYR:O	2.17	0.43
2:U:83:LEU:HD22	2:U:166:GLN:HB3	1.99	0.43
2:X:175:LEU:HD23	2:X:175:LEU:C	2.44	0.43
1:H:38:LYS:HB2	1:H:48:ILE:HD11	2.01	0.43
1:V:66:LYS:HB2	1:V:66:LYS:HE2	1.32	0.43
2:L:16:GLY:HA2	2:L:77:ASN:HD22	1.84	0.43
2:U:160:GLN:NE2	1:V:169:VAL:CG1	2.82	0.43
2:L:29:VAL:HG22	2:L:92:ASN:HB2	2.00	0.43
1:H:101:ASP:HB3	2:L:46:ALA:HB3	1.99	0.42
2:X:140:TYR:CG	2:X:141:PRO:HA	2.54	0.42
1:H:127:SER:C	1:H:129:LYS:N	2.77	0.42
2:X:48:ILE:HA	2:X:53:TYR:O	2.19	0.42
2:L:48:ILE:HA	2:L:53:TYR:O	2.20	0.42
2:U:145:ALA:HB3	2:U:197:THR:HB	2.02	0.42
1:V:12:VAL:CG1	1:V:18:VAL:CG1	2.93	0.42
1:V:59:TYR:CE1	1:V:69:LEU:HD13	2.55	0.42
1:Y:211:VAL:O	1:Y:211:VAL:CG2	2.67	0.42
1:Y:211:VAL:O	1:Y:211:VAL:HG22	2.19	0.42
2:L:29:VAL:HG23	2:L:92:ASN:HB3	2.02	0.42
2:L:193:ALA:HB2	2:L:208:SER:HB3	2.02	0.42
1:H:131:THR:HA	1:H:136:ALA:HA	2.02	0.42
2:L:183:LYS:O	2:L:187:GLU:HG2	2.20	0.42
1:V:127:SER:C	1:V:129:LYS:N	2.76	0.42
1:Y:12:VAL:O	1:Y:111:VAL:HA	2.19	0.42
1:H:20:ILE:HB	1:H:80:ILE:CG2	2.49	0.41
1:H:127:SER:O	1:H:129:LYS:N	2.53	0.41
1:H:139:GLY:HA2	1:H:154:TRP:CH2	2.55	0.41
1:Y:127:SER:O	1:Y:128:SER:C	2.62	0.41
2:L:33:VAL:HG21	2:L:71:PHE:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:145:ALA:O	2:L:196:VAL:HA	2.20	0.41
2:L:12:SER:HA	2:L:105:GLU:O	2.20	0.41
2:U:29:VAL:O	2:U:29:VAL:HG13	2.21	0.41
2:U:141:PRO:O	2:U:198:HIS:HE1	2.03	0.41
1:H:64:ARG:CG	1:H:64:ARG:HH11	2.34	0.41
2:X:35:TRP:CZ3	2:X:88:CYS:HB3	2.56	0.41
2:X:116:PHE:HD1	1:Y:130:SER:HA	1.85	0.41
2:U:186:TYR:HA	2:U:192:TYR:OH	2.21	0.41
2:X:150:VAL:O	2:X:151:ASP:HB2	2.20	0.41
1:H:47:TRP:CH2	1:H:49:GLY:HA2	2.56	0.41
1:H:86:THR:O	1:H:111:VAL:HG21	2.21	0.41
2:L:182:SER:O	2:L:183:LYS:C	2.64	0.41
1:V:189:LEU:HD12	1:V:189:LEU:HA	1.81	0.41
2:X:90:GLN:NE2	2:X:97:THR:OG1	2.54	0.41
1:Y:30:THR:CG2	1:Y:71:VAL:HG13	2.50	0.41
1:Y:98:PHE:CD1	1:Y:98:PHE:C	2.98	0.41
2:X:61:ARG:HD2	2:X:76:SER:O	2.21	0.41
2:X:164:THR:HG23	2:X:165:GLU:N	2.36	0.40
2:X:186:TYR:CE2	2:X:211:ARG:HD2	2.56	0.40
1:V:192:GLN:CD	1:V:192:GLN:H	2.30	0.40
1:H:37:VAL:HG22	1:H:47:TRP:HA	2.03	0.40
2:X:83:LEU:HD13	2:X:166:GLN:HB3	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:ASN:OD1	1:Y:23:ALA:CB[2_656]	1.68	0.52
1:H:100:GLY:N	1:Y:26:ALA:O[2_656]	2.05	0.15
1:H:100:GLY:CA	1:Y:26:ALA:O[2_656]	2.18	0.02

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	H	216/218 (99%)	199 (92%)	12 (6%)	5 (2%)	5	11
1	V	216/218 (99%)	205 (95%)	9 (4%)	2 (1%)	14	31
1	Y	216/218 (99%)	201 (93%)	12 (6%)	3 (1%)	9	21
2	L	211/213 (99%)	200 (95%)	10 (5%)	1 (0%)	24	45
2	U	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	24	45
2	X	211/213 (99%)	201 (95%)	9 (4%)	1 (0%)	24	45
All	All	1281/1293 (99%)	1208 (94%)	60 (5%)	13 (1%)	12	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	26	ALA
1	H	100(C)	PHE
1	V	26	ALA
1	Y	26	ALA
1	H	4(A)	LEU
2	U	211	ARG
2	X	211	ARG
1	Y	128	SER
1	Y	189	LEU
1	H	128	SER
2	L	211	ARG
1	V	189	LEU
1	H	100	GLY

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	H	181/181 (100%)	148 (82%)	33 (18%)	2	4
1	V	181/181 (100%)	148 (82%)	33 (18%)	2	4
1	Y	181/181 (100%)	144 (80%)	37 (20%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	181/181 (100%)	156 (86%)	25 (14%)	3	8
2	U	181/181 (100%)	151 (83%)	30 (17%)	2	5
2	X	181/181 (100%)	155 (86%)	26 (14%)	3	7
All	All	1086/1086 (100%)	902 (83%)	184 (17%)	2	5

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	7	SER
1	H	12	VAL
1	H	18	VAL
1	H	19	LYS
1	H	25	SER
1	H	27	TYR
1	H	29	ILE
1	H	31	ASP
1	H	62	LYS
1	H	64	ARG
1	H	66	LYS
1	H	68	THR
1	H	71	VAL
1	H	73	THR
1	H	74	SER
1	H	76	SER
1	H	84	SER
1	H	95	CYS
1	H	117	LYS
1	H	129	LYS
1	H	130	SER
1	H	131	THR
1	H	150	VAL
1	H	175	LEU
1	H	179	SER
1	H	189	LEU
1	H	191	THR
1	H	197	ASN
1	H	199	ASN
1	H	201	LYS
1	H	209	LYS
1	H	211	VAL
1	H	216	CYS

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Mol	Chain	Res	Type
2	L	1	LEU
2	L	1(A)	ASP
2	L	9	SER
2	L	19	VAL
2	L	31	THR
2	L	48	ILE
2	L	54	ARG
2	L	56	SER
2	L	67	SER
2	L	81	GLU
2	L	83	LEU
2	L	90	GLN
2	L	93	ILE
2	L	105	GLU
2	L	106	ILE
2	L	108	ARG
2	L	110	VAL
2	L	123	GLU
2	L	137	ASN
2	L	156	SER
2	L	160	GLN
2	L	164	THR
2	L	168	SER
2	L	183	LYS
2	L	196	VAL
2	U	1	LEU
2	U	1(A)	ASP
2	U	7	SER
2	U	9	SER
2	U	12	SER
2	U	14	SER
2	U	19	VAL
2	U	29	VAL
2	U	56	SER
2	U	67	SER
2	U	81	GLU
2	U	83	LEU
2	U	90	GLN
2	U	108	ARG
2	U	110	VAL
2	U	114	SER
2	U	123	GLU

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Mol	Chain	Res	Type
2	U	137	ASN
2	U	154	LEU
2	U	156	SER
2	U	164	THR
2	U	183	LYS
2	U	194	CYS
2	U	196	VAL
2	U	197	THR
2	U	199	GLN
2	U	203	SER
2	U	207	LYS
2	U	208	SER
2	U	211	ARG
1	V	4	LEU
1	V	4(A)	LEU
1	V	17	SER
1	V	18	VAL
1	V	19	LYS
1	V	21	SER
1	V	43	ASP
1	V	64	ARG
1	V	66	LYS
1	V	74	SER
1	V	84	SER
1	V	95	CYS
1	V	116	THR
1	V	117	LYS
1	V	129	LYS
1	V	131	THR
1	V	135	THR
1	V	143	LYS
1	V	160	THR
1	V	161	SER
1	V	172	SER
1	V	175	LEU
1	V	177	SER
1	V	179	SER
1	V	183	THR
1	V	189	LEU
1	V	191	THR
1	V	193	THR
1	V	199	ASN

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Mol	Chain	Res	Type
1	V	209	LYS
1	V	212	GLU
1	V	214	LYS
1	V	215	SER
2	X	7	SER
2	X	9	SER
2	X	11	MET
2	X	18	ARG
2	X	19	VAL
2	X	22	THR
2	X	27	GLN
2	X	45	LYS
2	X	48	ILE
2	X	60	ASP
2	X	63	THR
2	X	77	ASN
2	X	83	LEU
2	X	90	GLN
2	X	102	THR
2	X	108	ARG
2	X	110	VAL
2	X	123	GLU
2	X	127	SER
2	X	129	THR
2	X	163	VAL
2	X	164	THR
2	X	196	VAL
2	X	197	THR
2	X	199	GLN
2	X	205	VAL
1	Y	4	LEU
1	Y	4(A)	LEU
1	Y	7	SER
1	Y	12	VAL
1	Y	19	LYS
1	Y	29	ILE
1	Y	32	PHE
1	Y	43	ASP
1	Y	44	SER
1	Y	51	ILE
1	Y	61	GLN
1	Y	64	ARG

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Mol	Chain	Res	Type
1	Y	66	LYS
1	Y	80	ILE
1	Y	81	HIS
1	Y	83	ASN
1	Y	88	GLU
1	Y	115	SER
1	Y	127	SER
1	Y	130	SER
1	Y	143	LYS
1	Y	150	VAL
1	Y	151	THR
1	Y	161	SER
1	Y	172	SER
1	Y	175	LEU
1	Y	177	SER
1	Y	179	SER
1	Y	183	THR
1	Y	189	LEU
1	Y	191	THR
1	Y	195	ILE
1	Y	211	VAL
1	Y	212	GLU
1	Y	214	LYS
1	Y	215	SER
1	Y	216	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	41	HIS
1	H	54	ASN
1	H	192	GLN
1	H	200	HIS
2	L	2	ASN
2	L	28	ASN
2	L	77	ASN
2	L	89	GLN
2	L	137	ASN
2	L	160	GLN
2	L	198	HIS
2	L	199	GLN
2	U	32	ASN

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Mol	Chain	Res	Type
2	U	77	ASN
2	U	90	GLN
2	U	92	ASN
2	U	160	GLN
2	U	198	HIS
1	V	164	HIS
1	V	192	GLN
1	V	200	HIS
2	X	2	ASN
2	X	38	GLN
2	X	77	ASN
2	X	137	ASN
2	X	198	HIS
1	Y	39	GLN
1	Y	81	HIS
1	Y	164	HIS
1	Y	171	GLN
1	Y	192	GLN
1	Y	199	ASN
1	Y	200	HIS

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 [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.