



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:04 PM UTC

PDB ID : 1K8D / pdb_00001k8d
Title : crystal structure of the non-classical MHC class Ib Qa-2 complexed with a self peptide
Authors : He, X.; Tabaczewski, P.; Ho, J.; Stroynowski, I.; Garcia, K.C.
Deposited on : 2001-10-23
Resolution : 2.30 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

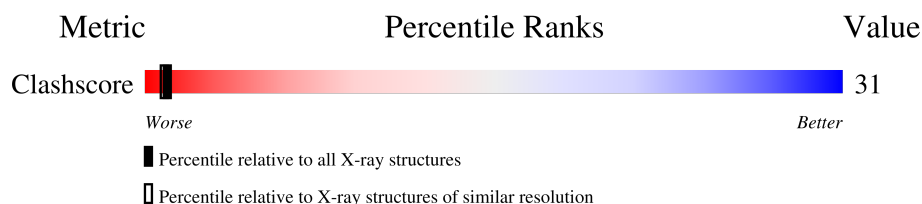
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)

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	A	274	 52% 46% .
2	B	99	 49% 51%
3	P	9	 56% 44%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3399 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 QA-2 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2226	1400	395	420	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	GLU	GLN	SEE REMARK 999	UNP P14429

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			79	52	14	12	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	179	Total	O	0	0
			179	179		
4	B	82	Total	O	0	0
			82	82		
4	P	12	Total	O	0	0
			12	12		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.92Å 56.18Å 119.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	97.6 (50.00-2.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3399	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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	A	0.43	0/2289	0.93	11/3104 (0.4%)
2	B	0.54	0/847	0.98	1/1148 (0.1%)
3	P	0.45	0/80	0.88	0/104
All	All	0.46	0/3216	0.95	12/4356 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLY	CA-C-N	8.31	127.88	119.24
1	A	56	GLY	C-N-CA	8.31	127.88	119.24
1	A	186	LYS	N-CA-C	-7.28	95.76	108.20
1	A	228	MET	N-CA-C	6.03	118.54	108.96
1	A	28	VAL	N-CA-C	-5.97	99.04	107.75
1	A	162	GLY	N-CA-C	5.74	115.43	110.21
1	A	14	ARG	CA-C-N	5.72	125.74	119.90
1	A	14	ARG	C-N-CA	5.72	125.74	119.90
2	B	75	THR	N-CA-C	5.62	120.27	113.41
1	A	181	ARG	N-CA-C	-5.51	103.23	110.33
1	A	69	GLY	N-CA-C	-5.32	106.33	112.50
1	A	29	ASP	CB-CA-C	-5.18	110.59	116.54

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	2226	0	2097	131	0
2	B	821	0	796	64	0
3	P	79	0	88	5	0
4	A	179	0	0	14	0
4	B	82	0	0	10	0
4	P	12	0	0	1	0
All	All	3399	0	2981	189	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 31.

All (189) 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:133:TRP:HB2	1:A:144:ARG:HD2	1.41	1.01
1:A:19:GLU:HG2	1:A:75:ARG:HE	1.37	0.89
2:B:39:MET:HE3	2:B:68:THR:HG23	1.53	0.88
1:A:19:GLU:CG	1:A:75:ARG:HE	1.87	0.87
1:A:12:VAL:HG22	1:A:94:THR:HG22	1.58	0.84
2:B:51:MET:HG3	2:B:64:ILE:HD11	1.59	0.83
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.64	0.80
1:A:230:LEU:HD21	1:A:243:LYS:HE3	1.64	0.79
2:B:39:MET:HE1	2:B:67:HIS:C	2.08	0.78
2:B:70:PHE:CE2	2:B:72:PRO:HG3	2.19	0.77
1:A:173:GLU:O	1:A:176:LYS:HG3	1.85	0.76
1:A:35:ARG:HH11	1:A:35:ARG:HG3	1.49	0.75
1:A:162:GLY:O	1:A:166:GLN:HG3	1.86	0.75
1:A:178:THR:O	1:A:181:ARG:HG2	1.86	0.74
2:B:48:LYS:O	2:B:68:THR:HG22	1.88	0.72
2:B:39:MET:CE	2:B:49:VAL:HG13	2.19	0.71
1:A:184:PRO:HB3	1:A:265:GLY:O	1.91	0.70
1:A:214:THR:HB	1:A:262:ASN:HB2	1.72	0.70
1:A:230:LEU:HD21	1:A:243:LYS:CE	2.22	0.69
2:B:39:MET:HE1	2:B:67:HIS:CA	2.22	0.69
2:B:98:ASP:O	2:B:99:MET:HG2	1.92	0.69
1:A:232:GLU:HG2	2:B:8:GLN:NE2	2.08	0.69
2:B:96:ASP:CG	2:B:99:MET:H	2.00	0.68
1:A:154:GLU:HG3	4:A:444:HOH:O	1.94	0.68
2:B:39:MET:CE	2:B:68:THR:HG23	2.23	0.67
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.77	0.67
1:A:34:VAL:HB	1:A:45:MET:HE2	1.77	0.67
1:A:48:ARG:HB3	1:A:48:ARG:HH11	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HD2	2:B:53:ASP:CG	2.20	0.66
1:A:65:GLN:HB2	4:A:393:HOH:O	1.95	0.66
2:B:19:LYS:HG3	4:B:164:HOH:O	1.96	0.65
1:A:121:ARG:HD2	4:A:450:HOH:O	1.95	0.65
2:B:97:ARG:HG3	4:B:149:HOH:O	1.97	0.65
1:A:45:MET:HG2	1:A:63:GLU:HB3	1.79	0.64
2:B:4:THR:HG22	2:B:86:SER:HB2	1.79	0.64
2:B:89:GLU:HG2	4:B:155:HOH:O	1.97	0.64
1:A:157:GLN:O	1:A:161:GLU:HG3	1.97	0.64
1:A:19:GLU:HG2	1:A:75:ARG:NE	2.10	0.63
1:A:227:ASP:HB3	4:A:405:HOH:O	1.97	0.63
1:A:19:GLU:CG	1:A:75:ARG:NE	2.61	0.63
1:A:48:ARG:HB3	1:A:48:ARG:NH1	2.14	0.63
1:A:12:VAL:HG21	2:B:33:PRO:HG3	1.81	0.62
1:A:35:ARG:C	1:A:45:MET:HE3	2.23	0.62
2:B:38:GLN:CD	2:B:45:LYS:HE2	2.25	0.62
1:A:178:THR:HA	1:A:181:ARG:HD3	1.82	0.60
2:B:49:VAL:HG22	2:B:68:THR:CG2	2.31	0.60
1:A:35:ARG:HG3	1:A:35:ARG:NH1	2.16	0.60
1:A:48:ARG:HH11	1:A:48:ARG:CB	2.13	0.60
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.83	0.60
1:A:14:ARG:NH2	1:A:39:ASP:OD1	2.29	0.59
1:A:35:ARG:NH2	1:A:37:ASP:HB2	2.19	0.58
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.85	0.58
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.39	0.57
2:B:96:ASP:HB3	2:B:99:MET:HA	1.86	0.57
1:A:35:ARG:NH2	1:A:37:ASP:OD2	2.38	0.57
1:A:258:THR:OG1	1:A:271:THR:HG23	2.05	0.57
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.87	0.56
1:A:191:HIS:HE1	1:A:254:GLU:OE2	1.88	0.56
2:B:1:ILE:HA	4:B:169:HOH:O	2.05	0.56
1:A:226:GLN:HG2	4:A:401:HOH:O	2.06	0.55
1:A:14:ARG:HH22	1:A:39:ASP:CG	2.15	0.55
1:A:103:MET:CE	1:A:169:ARG:HG2	2.37	0.55
1:A:232:GLU:HG2	2:B:8:GLN:HE21	1.70	0.55
2:B:87:MET:SD	2:B:91:LYS:HB2	2.47	0.55
1:A:97:TRP:HE1	1:A:114:LEU:HG	1.72	0.55
1:A:218:GLN:HB2	1:A:222:GLU:O	2.06	0.55
1:A:183:ASP:HB3	4:A:373:HOH:O	2.07	0.54
1:A:103:MET:HE1	1:A:169:ARG:HG2	1.90	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:NH1	4:A:388:HOH:O	2.41	0.54
2:B:12:ARG:NH1	2:B:22:ILE:HD12	2.23	0.54
1:A:167:SER:HB2	1:A:171:TYR:CE2	2.44	0.53
1:A:19:GLU:HG2	1:A:75:ARG:HH21	1.72	0.53
2:B:49:VAL:HA	2:B:68:THR:HG22	1.90	0.53
3:P:3:MET:HG2	3:P:5:HIS:H	1.74	0.53
1:A:71:GLU:CD	1:A:75:ARG:HH12	2.18	0.52
1:A:114:LEU:HD12	3:P:3:MET:HE1	1.90	0.52
1:A:230:LEU:HD23	1:A:231:VAL:O	2.10	0.52
2:B:7:ILE:HD12	2:B:91:LYS:HG2	1.92	0.52
2:B:51:MET:HG3	2:B:64:ILE:CD1	2.37	0.52
1:A:170:ARG:O	1:A:173:GLU:HB2	2.10	0.52
2:B:1:ILE:HG13	4:B:169:HOH:O	2.10	0.52
2:B:1:ILE:HD13	2:B:3:LYS:HE3	1.92	0.51
1:A:144:ARG:HG2	4:A:388:HOH:O	2.10	0.51
1:A:190:THR:OG1	1:A:192:HIS:HE1	1.94	0.51
1:A:194:ARG:HG2	1:A:194:ARG:HH11	1.76	0.51
1:A:22:PHE:HB3	1:A:38:SER:HB3	1.93	0.51
1:A:206:LEU:HD12	4:A:394:HOH:O	2.10	0.50
1:A:117:ALA:HA	1:A:121:ARG:O	2.11	0.50
2:B:51:MET:CG	2:B:64:ILE:HD11	2.36	0.50
2:B:19:LYS:HB3	4:B:112:HOH:O	2.11	0.50
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.77	0.50
1:A:258:THR:HA	1:A:272:LEU:O	2.12	0.50
1:A:191:HIS:CE1	1:A:199:VAL:HG21	2.47	0.50
1:A:234:ARG:NH1	2:B:99:MET:SD	2.81	0.50
1:A:273:ARG:O	1:A:274:TRP:CB	2.61	0.49
1:A:178:THR:O	1:A:181:ARG:NH1	2.44	0.49
1:A:19:GLU:HG3	1:A:75:ARG:HE	1.74	0.49
1:A:144:ARG:O	1:A:148:GLU:HG3	2.12	0.49
1:A:187:ALA:HA	1:A:204:TRP:O	2.12	0.49
2:B:59:ASP:O	2:B:60:TRP:HB2	2.12	0.49
1:A:7:TYR:CD2	3:P:2:LEU:HD23	2.47	0.49
1:A:19:GLU:HG3	1:A:75:ARG:NE	2.28	0.49
1:A:50:ARG:HD3	4:A:415:HOH:O	2.13	0.49
1:A:165:MET:O	1:A:169:ARG:HG3	2.14	0.48
2:B:38:GLN:OE1	2:B:81:ARG:NH2	2.41	0.48
2:B:48:LYS:HE2	2:B:50:GLU:OE1	2.13	0.48
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.95	0.48
1:A:169:ARG:O	1:A:173:GLU:HG3	2.13	0.48
2:B:13:HIS:HB3	2:B:14:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:HG2	2:B:48:LYS:H	1.79	0.48
1:A:35:ARG:O	1:A:45:MET:HE3	2.14	0.48
2:B:19:LYS:CG	4:B:164:HOH:O	2.59	0.48
2:B:99:MET:HE1	4:B:145:HOH:O	2.14	0.48
1:A:9:HIS:HB2	1:A:97:TRP:HB3	1.95	0.47
1:A:35:ARG:C	1:A:45:MET:CE	2.87	0.47
2:B:49:VAL:HG22	2:B:68:THR:HG21	1.94	0.47
1:A:25:VAL:HG11	4:A:316:HOH:O	2.14	0.47
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.50	0.47
1:A:191:HIS:CE1	1:A:254:GLU:OE2	2.67	0.47
1:A:249:VAL:HG13	1:A:250:PRO:HD2	1.96	0.47
1:A:128:GLU:HA	4:A:276:HOH:O	2.15	0.47
1:A:230:LEU:CD2	1:A:243:LYS:HE3	2.41	0.47
1:A:141:GLN:O	1:A:145:ARG:HG3	2.15	0.46
2:B:1:ILE:CD1	2:B:3:LYS:HE3	2.46	0.46
1:A:247:VAL:HG13	1:A:249:VAL:HG23	1.98	0.46
2:B:98:ASP:C	2:B:99:MET:HG2	2.40	0.46
1:A:218:GLN:HG2	1:A:260:HIS:CD2	2.50	0.45
2:B:50:GLU:HB2	2:B:67:HIS:CE1	2.50	0.45
3:P:6:ILE:HD11	4:P:19:HOH:O	2.15	0.45
1:A:189:VAL:HG23	1:A:272:LEU:HB3	1.98	0.45
1:A:45:MET:HG2	1:A:63:GLU:CB	2.44	0.45
1:A:103:MET:HE3	1:A:168:LEU:HD23	1.99	0.45
2:B:35:ILE:HD11	2:B:82:VAL:CG1	2.47	0.45
2:B:39:MET:HE1	2:B:67:HIS:HA	1.97	0.45
1:A:111:ARG:NH1	1:A:128:GLU:OE1	2.50	0.44
1:A:21:TRP:CZ2	1:A:23:ILE:HD13	2.52	0.44
1:A:21:TRP:CH2	1:A:23:ILE:HD13	2.52	0.44
2:B:16:GLU:HG2	2:B:19:LYS:HE3	1.99	0.44
1:A:147:TRP:CD1	1:A:152:ILE:HD12	2.53	0.44
2:B:29:GLN:HA	2:B:61:SER:OG	2.18	0.44
2:B:33:PRO:O	2:B:54:MET:HE1	2.17	0.44
1:A:4:SER:HA	1:A:101:CYS:O	2.18	0.44
1:A:217:TRP:CD2	1:A:259:CYS:HB3	2.53	0.44
1:A:255:GLN:NE2	1:A:255:GLN:C	2.75	0.44
1:A:3:HIS:HA	1:A:29:ASP:OD1	2.17	0.43
1:A:35:ARG:HG2	1:A:36:PHE:N	2.33	0.43
2:B:81:ARG:HD2	4:B:165:HOH:O	2.17	0.43
1:A:231:VAL:HG13	1:A:232:GLU:O	2.18	0.43
1:A:237:GLY:HA3	4:B:102:HOH:O	2.17	0.43
1:A:119:GLU:O	2:B:1:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.52	0.43
1:A:185:PRO:HG3	1:A:208:PHE:HB3	2.00	0.43
1:A:195:SER:OG	1:A:198:ALA:HB3	2.19	0.43
1:A:229:GLU:O	1:A:245:ALA:HA	2.19	0.43
2:B:12:ARG:CZ	2:B:22:ILE:HD12	2.49	0.43
2:B:96:ASP:CG	2:B:99:MET:N	2.75	0.43
1:A:35:ARG:NH2	4:A:321:HOH:O	2.52	0.42
1:A:64:THR:O	1:A:68:LYS:HG3	2.19	0.42
2:B:49:VAL:HA	2:B:68:THR:CG2	2.49	0.42
2:B:58:LYS:HG2	2:B:59:ASP:H	1.84	0.42
1:A:103:MET:HG3	1:A:165:MET:HE1	2.02	0.42
2:B:58:LYS:CG	2:B:59:ASP:N	2.83	0.42
1:A:118:TYR:CD2	1:A:119:GLU:HG2	2.55	0.42
1:A:273:ARG:O	1:A:274:TRP:HB3	2.19	0.42
1:A:48:ARG:HH11	1:A:48:ARG:CA	2.32	0.42
1:A:184:PRO:HB3	1:A:265:GLY:C	2.45	0.42
1:A:19:GLU:HG2	1:A:75:ARG:NH2	2.34	0.41
1:A:114:LEU:CD1	3:P:3:MET:HE1	2.50	0.41
1:A:203:CYS:O	1:A:244:TRP:HA	2.20	0.41
1:A:175:GLY:O	1:A:176:LYS:C	2.63	0.41
2:B:11:SER:HA	2:B:22:ILE:O	2.20	0.41
1:A:15:PRO:HG3	1:A:90:GLY:C	2.45	0.41
1:A:48:ARG:HA	1:A:48:ARG:HD2	1.93	0.41
1:A:114:LEU:HD23	1:A:114:LEU:C	2.45	0.41
1:A:159:TYR:CD1	1:A:163:THR:HB	2.56	0.41
1:A:12:VAL:HG21	2:B:33:PRO:CG	2.49	0.41
1:A:19:GLU:HG3	1:A:20:PRO:CD	2.48	0.41
1:A:129:ASP:O	1:A:130:LEU:HB2	2.21	0.41
1:A:130:LEU:HB3	1:A:157:GLN:HB2	2.02	0.41
1:A:230:LEU:HD21	1:A:243:LYS:NZ	2.35	0.41
1:A:229:GLU:HB3	1:A:246:SER:OG	2.20	0.41
1:A:266:LEU:HA	1:A:267:PRO:HD3	1.95	0.41
2:B:36:GLU:OE2	2:B:38:GLN:NE2	2.53	0.41
2:B:97:ARG:HG3	2:B:97:ARG:H	1.73	0.41
1:A:182:THR:HG23	1:A:210:PRO:HD3	2.03	0.40
1:A:252:GLY:N	1:A:254:GLU:OE1	2.52	0.40
2:B:4:THR:HA	2:B:86:SER:OG	2.21	0.40
1:A:79:ARG:NH1	4:A:309:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides 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

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.