



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:41 pm BST

PDB ID : 1TD0  
Title : Viral capsid protein SHP at pH 5.5  
Authors : Chang, C.; Forrer, P.; Ott, D.; Wlodawer, A.; Plueckthun, A.  
Deposited on : 2004-05-21  
Resolution : 1.95 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](mailto: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.

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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

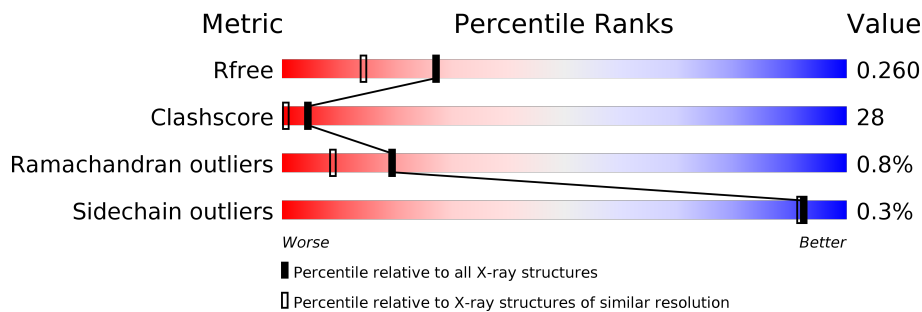
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	114	62% (green), 27% (yellow), 11% (grey)
1	B	114	61% (green), 28% (yellow), 11% (grey)
1	C	114	58% (green), 30% (yellow), 11% (grey)
1	D	114	51% (green), 38% (yellow), 10% (grey)

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3536 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 Head decoration protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	102	Total 727	C 461	N 120	O 145	S 1	0	0	0
1	B	102	Total 727	C 461	N 120	O 145	S 1	0	0	0
1	C	101	Total 722	C 458	N 119	O 144	S 1	0	0	0
1	D	103	Total 735	C 467	N 121	O 146	S 1	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total 150	O 150	0	0
2	B	166	Total 166	O 166	0	0
2	C	164	Total 164	O 164	0	0
2	D	145	Total 145	O 145	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.48Å 57.48Å 101.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.74 – 1.95 28.74 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (28.74-1.95) 96.2 (28.74-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.229 , 0.260 0.230 , 0.260	Depositor DCC
$R_{free}$ test set	1316 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 85.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.480 for -h,-k,l 0.437 for h,-h-k,-l 0.438 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.36	0/745	0.59	0/1019
1	B	0.35	0/745	0.58	0/1019
1	C	0.34	0/740	0.58	0/1012
1	D	0.35	0/753	0.59	0/1030
All	All	0.35	0/2983	0.58	0/4080

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	727	0	695	37	0
1	B	727	0	695	43	0
1	C	722	0	693	41	0
1	D	735	0	706	60	0
2	A	150	0	0	12	0
2	B	166	0	0	18	0
2	C	164	0	0	20	0
2	D	145	0	0	36	0
All	All	3536	0	2789	162	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 28.

All (162) 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:D:614:ILE:H	1:D:614:ILE:HD12	1.05	1.08
1:C:414:ILE:HG13	1:D:614:ILE:HG12	1.39	1.02
1:D:641:MET:HA	2:D:1827:HOH:O	1.58	1.01
1:B:214:ILE:HG13	2:B:1702:HOH:O	1.68	0.94
1:D:614:ILE:H	1:D:614:ILE:CD1	1.82	0.93
1:D:660:ALA:HA	2:D:1976:HOH:O	1.67	0.92
1:D:664:LEU:HG	2:D:1973:HOH:O	1.74	0.86
1:D:614:ILE:HD12	1:D:614:ILE:N	1.91	0.85
1:B:250:VAL:HG22	2:B:1577:HOH:O	1.76	0.85
1:C:440:LEU:HB3	2:C:1906:HOH:O	1.79	0.81
1:B:291:PRO:HG2	1:B:294:VAL:HB	1.64	0.79
1:D:691:PRO:HG2	1:D:694:VAL:HB	1.64	0.79
1:C:491:PRO:HG2	1:C:494:VAL:HB	1.65	0.79
1:D:676:THR:HB	2:D:1979:HOH:O	1.82	0.78
1:A:91:PRO:HG2	1:A:94:VAL:HB	1.64	0.78
1:C:414:ILE:H	1:C:414:ILE:HD12	1.49	0.78
1:C:414:ILE:CG1	1:D:614:ILE:HG12	2.12	0.77
1:A:37:LEU:HD11	1:B:214:ILE:CG2	2.14	0.77
1:C:414:ILE:H	1:C:414:ILE:CD1	1.97	0.77
1:C:476:THR:HB	2:C:1855:HOH:O	1.83	0.77
1:D:679:LYS:NZ	2:D:1602:HOH:O	2.17	0.77
1:D:661:VAL:HG13	2:D:1827:HOH:O	1.84	0.76
1:D:661:VAL:HG22	2:D:1827:HOH:O	1.84	0.76
1:B:249:LEU:HD22	2:B:1446:HOH:O	1.84	0.76
1:B:217:GLY:HA3	1:B:282:THR:HB	1.69	0.75
1:C:417:GLY:HA3	1:C:482:THR:HB	1.69	0.75
1:D:617:GLY:HA3	1:D:682:THR:HB	1.69	0.75
1:A:76:THR:HB	2:A:1972:HOH:O	1.85	0.74
1:C:460:ALA:HB1	2:C:1857:HOH:O	1.87	0.73
1:A:17:GLY:HA3	1:A:82:THR:HB	1.69	0.73
1:A:60:ALA:HB1	2:A:1613:HOH:O	1.88	0.73
1:A:14:ILE:N	1:A:14:ILE:HD12	2.04	0.72
1:A:14:ILE:HD13	1:B:237:LEU:CD1	2.19	0.72
1:D:636:ALA:HA	2:D:1973:HOH:O	1.90	0.71
1:D:641:MET:HB3	2:D:1976:HOH:O	1.91	0.71
1:C:414:ILE:N	1:C:414:ILE:HD12	2.07	0.69
1:D:622:HIS:HB3	2:D:1920:HOH:O	1.92	0.69
1:A:14:ILE:HG12	1:B:214:ILE:HB	1.74	0.69
1:A:37:LEU:HD11	1:B:214:ILE:HG22	1.75	0.68
1:D:681:GLY:HA3	2:D:1749:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:618:ASN:ND2	2:D:1586:HOH:O	2.26	0.68
1:C:450:VAL:HG13	2:C:1815:HOH:O	1.97	0.65
1:A:37:LEU:HD11	1:B:214:ILE:HG21	1.79	0.65
1:A:14:ILE:HD11	1:B:287:ALA:HB1	1.79	0.65
1:C:414:ILE:HG13	1:D:614:ILE:CG1	2.24	0.65
1:B:250:VAL:HG13	2:B:1706:HOH:O	1.97	0.64
1:B:296:GLU:HB2	2:B:1090:HOH:O	1.97	0.64
1:C:508:LEU:HB3	2:C:1984:HOH:O	1.97	0.63
1:D:709:SER:HA	2:D:1770:HOH:O	1.99	0.63
1:C:448:LYS:HB2	2:C:1815:HOH:O	1.99	0.63
1:C:510:HIS:HB3	2:C:1969:HOH:O	1.98	0.63
1:A:81:GLY:HA3	2:A:1760:HOH:O	1.99	0.62
1:B:248:LYS:HB2	2:B:1706:HOH:O	1.98	0.62
1:B:252:TRP:CZ2	1:B:254:GLY:HA2	2.36	0.61
1:C:452:TRP:CZ2	1:C:454:GLY:HA2	2.36	0.61
1:C:465:VAL:HB	2:C:1855:HOH:O	1.99	0.61
1:C:456:LYS:HE3	2:C:1518:HOH:O	2.00	0.60
1:B:214:ILE:HD11	1:B:237:LEU:HD22	1.84	0.59
1:C:483:PHE:HB2	2:C:1969:HOH:O	2.01	0.59
1:D:616:ALA:HB1	1:D:713:LEU:HB2	1.84	0.59
1:B:256:LYS:HE3	2:B:1490:HOH:O	2.01	0.59
1:A:52:TRP:CZ2	1:A:54:GLY:HA2	2.38	0.59
1:B:216:ALA:HB3	2:B:1076:HOH:O	2.01	0.59
1:B:272:GLU:HB2	2:B:1747:HOH:O	2.03	0.59
1:D:653:ASP:HB2	2:D:1964:HOH:O	2.03	0.58
1:D:674:ALA:HB1	2:D:1647:HOH:O	2.03	0.58
1:C:437:LEU:CD1	1:D:614:ILE:HD13	2.32	0.58
1:D:651:VAL:HG22	2:D:1995:HOH:O	2.02	0.58
1:D:652:TRP:CZ2	1:D:654:GLY:HA2	2.39	0.58
1:A:65:VAL:HB	2:A:1972:HOH:O	2.05	0.57
1:D:665:VAL:HB	2:D:1979:HOH:O	2.04	0.56
1:A:108:LEU:HB3	2:A:1667:HOH:O	2.05	0.56
1:B:265:VAL:HG23	1:B:277:TYR:HA	1.88	0.56
1:D:679:LYS:HE2	2:D:1920:HOH:O	2.05	0.56
1:C:416:ALA:HB3	2:C:1907:HOH:O	2.05	0.56
1:D:625:THR:HB	2:D:1647:HOH:O	2.06	0.55
1:A:14:ILE:HD11	1:B:287:ALA:CB	2.36	0.55
1:C:465:VAL:HG23	1:C:477:TYR:HA	1.89	0.55
1:A:51:VAL:HG22	2:A:1961:HOH:O	2.05	0.55
1:D:665:VAL:HG23	1:D:677:TYR:HA	1.89	0.54
1:D:615:PHE:C	1:D:617:GLY:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:THR:HG21	2:D:1995:HOH:O	2.06	0.54
1:D:667:PRO:HG2	2:D:1802:HOH:O	2.08	0.54
1:A:65:VAL:HG23	1:A:77:TYR:HA	1.89	0.54
1:D:696:GLU:HB2	2:D:1110:HOH:O	2.07	0.53
1:B:276:THR:HG23	2:B:1122:HOH:O	2.09	0.53
1:A:86:GLU:HG2	2:B:1105:HOH:O	2.09	0.53
1:D:694:VAL:HG21	2:D:1879:HOH:O	2.08	0.53
1:D:659:SER:O	2:D:1827:HOH:O	2.19	0.53
1:A:67:PRO:HG2	2:A:1709:HOH:O	2.09	0.52
1:A:14:ILE:HG23	1:A:87:ALA:CB	2.39	0.52
1:D:652:TRP:HB2	2:D:1976:HOH:O	2.10	0.52
1:B:269:GLU:HA	1:B:269:GLU:OE2	2.10	0.52
1:C:469:GLU:HA	1:C:469:GLU:OE2	2.10	0.52
1:B:268:LEU:HD22	2:B:1747:HOH:O	2.10	0.51
1:D:621:ALA:HB2	2:D:1749:HOH:O	2.09	0.51
1:A:34:THR:HG21	2:A:1961:HOH:O	2.09	0.51
1:C:487:ALA:HB1	1:D:614:ILE:HD11	1.91	0.51
1:A:69:GLU:HA	1:A:69:GLU:OE2	2.11	0.51
1:D:669:GLU:HA	1:D:669:GLU:OE2	2.11	0.51
1:A:21:ALA:HB2	2:A:1760:HOH:O	2.11	0.51
1:A:37:LEU:CD1	1:B:214:ILE:HG22	2.40	0.50
1:B:311:ALA:HA	2:B:1860:HOH:O	2.11	0.50
1:B:243:ASP:N	2:B:1577:HOH:O	2.44	0.50
1:A:44:GLU:HB3	2:C:1569:HOH:O	2.12	0.49
1:D:666:LEU:N	2:D:1973:HOH:O	2.46	0.49
1:A:11:GLU:HA	1:B:286:GLU:O	2.12	0.49
1:C:475:LEU:C	1:C:475:LEU:HD12	2.33	0.49
1:D:615:PHE:O	1:D:617:GLY:N	2.40	0.49
1:C:418:ASN:HB2	2:C:1601:HOH:O	2.13	0.49
1:A:15:PHE:C	1:A:17:GLY:H	2.16	0.48
1:B:275:LEU:HD12	1:B:275:LEU:C	2.34	0.48
1:A:75:LEU:HD12	1:A:75:LEU:C	2.34	0.48
1:C:482:THR:HG22	2:C:1907:HOH:O	2.14	0.47
1:D:635:PRO:O	1:D:664:LEU:HD23	2.14	0.47
1:D:675:LEU:C	1:D:675:LEU:HD12	2.35	0.47
1:C:472:GLU:N	1:C:472:GLU:OE2	2.46	0.47
1:B:272:GLU:OE2	1:B:272:GLU:N	2.45	0.47
1:D:666:LEU:N	2:D:1979:HOH:O	2.47	0.47
1:D:672:GLU:N	1:D:672:GLU:OE2	2.47	0.47
1:C:420:PRO:HB3	2:D:1802:HOH:O	2.15	0.47
1:A:35:PRO:O	1:A:64:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE2	1:A:72:GLU:N	2.48	0.46
1:C:435:PRO:O	1:C:464:LEU:HD23	2.15	0.46
1:B:282:THR:HG22	2:B:1076:HOH:O	2.15	0.46
1:D:665:VAL:HA	2:D:1946:HOH:O	2.15	0.45
2:C:1748:HOH:O	1:D:686:GLU:HG2	2.16	0.45
1:D:678:TYR:HE1	2:D:1946:HOH:O	1.99	0.45
1:A:14:ILE:HD13	1:B:237:LEU:HD11	1.98	0.45
1:B:235:PRO:O	1:B:264:LEU:HD23	2.15	0.45
1:D:694:VAL:HG11	2:D:1879:HOH:O	2.16	0.45
1:C:486:GLU:O	1:D:611:GLU:HA	2.17	0.45
1:D:640:LEU:C	2:D:1976:HOH:O	2.56	0.44
2:A:1709:HOH:O	1:B:220:PRO:HB3	2.17	0.44
1:C:487:ALA:CB	1:D:614:ILE:HD11	2.48	0.44
1:C:496:GLU:HB2	2:C:1087:HOH:O	2.18	0.44
1:B:213:ARG:HA	2:B:1295:HOH:O	2.18	0.44
1:D:708:LEU:HB3	2:D:1908:HOH:O	2.17	0.44
1:A:66:LEU:N	2:A:1972:HOH:O	2.49	0.43
1:B:214:ILE:HD13	1:B:287:ALA:HB1	2.00	0.43
1:B:240:LEU:C	2:B:1446:HOH:O	2.57	0.43
1:C:466:LEU:HA	2:C:1612:HOH:O	2.18	0.43
1:C:449:LEU:HB3	2:C:1906:HOH:O	2.19	0.43
1:C:466:LEU:N	2:C:1855:HOH:O	2.51	0.43
1:B:214:ILE:HD11	1:B:237:LEU:CD2	2.49	0.43
1:C:414:ILE:HD13	1:D:637:LEU:CD1	2.49	0.42
1:B:213:ARG:C	1:B:215:PHE:N	2.72	0.42
1:D:703:PHE:HD1	2:D:1770:HOH:O	2.02	0.42
1:A:96:GLU:HB2	2:A:1144:HOH:O	2.19	0.41
1:D:710:HIS:CD2	2:D:1770:HOH:O	2.73	0.41
1:B:220:PRO:HG3	2:B:1633:HOH:O	2.19	0.41
1:C:415:PHE:C	1:C:417:GLY:H	2.24	0.41
1:B:252:TRP:CH2	1:B:254:GLY:HA2	2.56	0.41
1:C:452:TRP:CH2	1:C:454:GLY:HA2	2.56	0.41
1:C:493:SER:CA	2:C:1569:HOH:O	2.68	0.41
1:D:616:ALA:O	1:D:713:LEU:HD12	2.20	0.41
1:A:14:ILE:CD1	1:B:287:ALA:HB1	2.49	0.41
1:D:615:PHE:C	1:D:617:GLY:N	2.73	0.41
1:B:244:GLU:OE1	1:B:244:GLU:HA	2.21	0.40
1:A:14:ILE:HG22	1:A:14:ILE:O	2.20	0.40
1:C:444:GLU:OE1	1:C:444:GLU:HA	2.21	0.40
1:A:52:TRP:CH2	1:A:54:GLY:HA2	2.57	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	100/114 (88%)	98 (98%)	1 (1%)	1 (1%)	15	6
1	B	100/114 (88%)	98 (98%)	2 (2%)	0	100	100
1	C	99/114 (87%)	95 (96%)	4 (4%)	0	100	100
1	D	101/114 (89%)	96 (95%)	3 (3%)	2 (2%)	7	1
All	All	400/456 (88%)	387 (97%)	10 (2%)	3 (1%)	19	9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	616	ALA
1	D	614	ILE
1	A	16	ALA

### 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	72/87 (83%)	72 (100%)	0	100	100
1	B	72/87 (83%)	72 (100%)	0	100	100
1	C	72/87 (83%)	71 (99%)	1 (1%)	67	62
1	D	73/87 (84%)	73 (100%)	0	100	100
All	All	289/348 (83%)	288 (100%)	1 (0%)	92	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	414	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.