



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:18 pm BST

PDB ID : 1PH8  
Title : CRYSTAL STRUCTURE OF THE OXYTRICHA NOVA TELOMERE  
END-BINDING PROTEIN COMPLEXED WITH NONCOGNATE SSDNA  
GGGGTTTTGCGG  
Authors : Theobald, D.L.; Schultz, S.C.  
Deposited on : 2003-05-29  
Resolution : 2.36 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

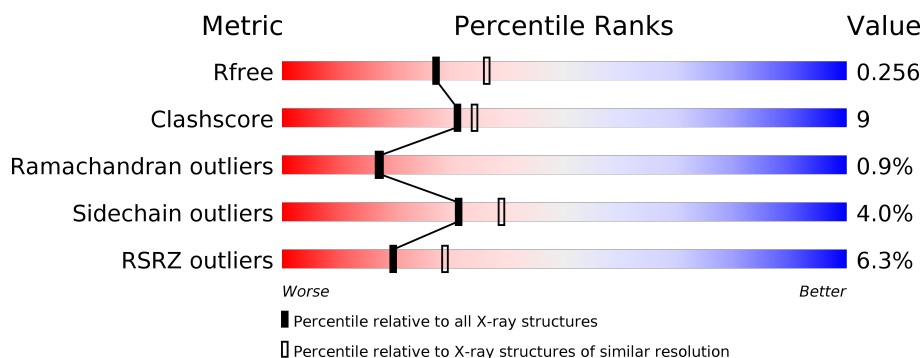
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\leq 5\%$ . 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	G	13	
1	H	13	
2	D	12	
3	A	460	
4	B	216	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6681 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 DNA chain called 5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*GP\*GP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	H	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			

- Molecule 2 is a DNA chain called 5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*CP\*GP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	P	0	0	0
			228	109	41	68	10			

- Molecule 3 is a protein called Telomere-binding protein alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	460	Total	C	N	O	S	0	0	0
			3706	2355	637	712	2			

- Molecule 4 is a protein called Telomere-binding protein beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	216	Total	C	N	O	S	0	0	0
			1733	1112	294	326	1			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Na	0	0
			1	1		
5	G	3	Total	Na	0	0
			3	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	32	Total O 32 32	0	0
7	D	28	Total O 28 28	0	0
7	H	36	Total O 36 36	0	0
7	A	336	Total O 336 336	0	0
7	B	71	Total O 71 71	0	0

### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: 5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*GP\*GP\*T)-3'

Chain G: 



- Molecule 1: 5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*GP\*GP\*T)-3'

Chain H: 




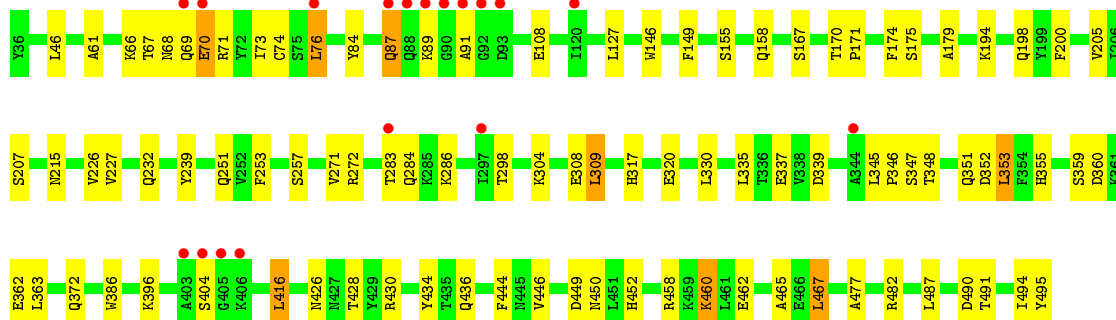
- Molecule 2: 5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*CP\*GP\*G)-3'

Chain D: 

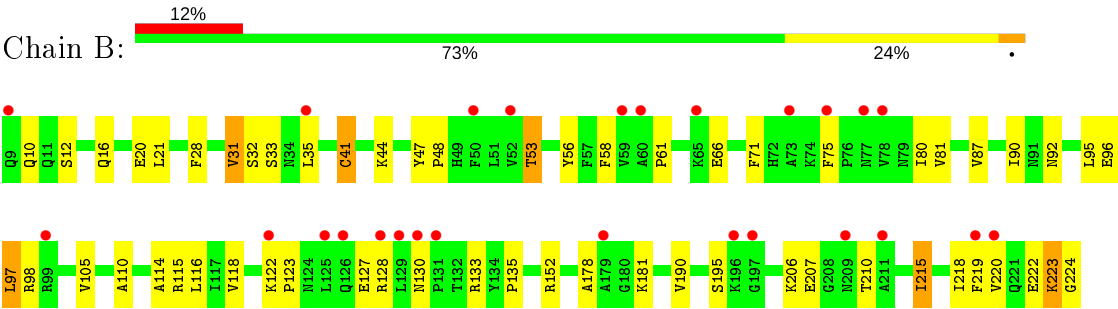


- Molecule 3: Telomere-binding protein alpha subunit

Chain A: 



- Molecule 4: Telomere-binding protein beta subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.47Å 93.47Å 423.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.90 – 2.36 29.90 – 2.36	Depositor EDS
% Data completeness (in resolution range)	83.8 (29.90-2.36) 83.9 (29.90-2.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.36Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.222 , 0.256 0.222 , 0.256	Depositor DCC
$R_{free}$ test set	3859 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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	G	0.70	0/284	0.72	0/440
1	H	0.64	0/284	0.72	0/440
2	D	1.11	0/255	0.99	1/394 (0.3%)
3	A	0.63	0/3777	0.64	0/5104
4	B	0.51	0/1771	0.52	0/2391
All	All	0.63	0/6371	0.64	1/8769 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	DG	O4'-C1'-N9	-5.02	104.49	108.00

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	G	253	0	138	2	0
1	H	253	0	138	4	0
2	D	228	0	127	8	0
3	A	3706	0	3699	56	0
4	B	1733	0	1718	41	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	3	0	0	0	0
5	H	1	0	0	0	0
6	A	1	0	0	0	0
7	A	336	0	0	3	2
7	B	71	0	0	2	0
7	D	28	0	0	1	0
7	G	32	0	0	0	0
7	H	36	0	0	1	0
All	All	6681	0	5820	108	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 9.

All (108) 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)
4:B:10:GLN:HE21	4:B:12:SER:H	1.07	0.97
4:B:80:ILE:HD12	4:B:218:ILE:HD11	1.63	0.81
4:B:41:CYS:HB3	4:B:53:THR:O	1.91	0.70
3:A:108:GLU:CD	3:A:108:GLU:H	1.96	0.70
3:A:345:LEU:HD12	3:A:346:PRO:HD2	1.77	0.67
3:A:339:ASP:HB2	3:A:490:ASP:HB3	1.76	0.66
3:A:155:SER:H	3:A:158:GLN:NE2	1.93	0.66
4:B:21:LEU:HD22	4:B:95:LEU:HB3	1.79	0.65
4:B:10:GLN:HE21	4:B:12:SER:N	1.88	0.64
3:A:284:GLN:HG3	3:A:330:LEU:HD12	1.79	0.64
4:B:10:GLN:HG2	4:B:16:GLN:HB2	1.80	0.64
4:B:10:GLN:NE2	4:B:12:SER:H	1.88	0.63
4:B:96:GLU:OE2	4:B:210:THR:HG22	1.99	0.63
4:B:220:VAL:HG13	4:B:224:GLY:HA2	1.81	0.63
2:D:12:DG:H2'	2:D:12:DG:N3	2.15	0.61
3:A:76:LEU:HD23	3:A:76:LEU:N	2.18	0.58
3:A:477:ALA:HB2	3:A:491:THR:HG21	1.85	0.58
3:A:194:LYS:O	3:A:198:GLN:HG3	2.02	0.58
3:A:149:PHE:CE2	3:A:171:PRO:HG3	2.39	0.57
3:A:200:PHE:CZ	3:A:205:VAL:HG11	2.39	0.57
4:B:20:GLU:HB3	4:B:31:VAL:HG23	1.87	0.57
4:B:90:ILE:HG23	4:B:118:VAL:HG13	1.88	0.56
4:B:178:ALA:HA	4:B:181:LYS:HD2	1.88	0.56
2:D:7:DT:C6	2:D:7:DT:H5'	2.41	0.55
4:B:81:VAL:HG23	4:B:222:GLU:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:98:ARG:HG3	4:B:115:ARG:HD2	1.89	0.55
3:A:335:LEU:HD22	3:A:467:LEU:HD23	1.87	0.55
4:B:71:PHE:CE1	4:B:123:PRO:HD3	2.42	0.54
3:A:67:THR:HG21	3:A:73:ILE:HD12	1.89	0.54
4:B:81:VAL:HG11	4:B:219:PHE:HD1	1.73	0.53
3:A:61:ALA:HB2	3:A:76:LEU:HB3	1.90	0.53
4:B:32:SER:HB2	4:B:35:LEU:HD12	1.92	0.52
4:B:206:LYS:O	4:B:206:LYS:HG3	2.08	0.51
3:A:215:ASN:HA	3:A:251:GLN:HG3	1.92	0.51
4:B:178:ALA:HB1	4:B:181:LYS:HB2	1.93	0.50
4:B:28:PHE:O	4:B:31:VAL:HG12	2.12	0.50
3:A:66:LYS:HE2	3:A:68:ASN:O	2.11	0.49
1:G:11:DG:N3	1:G:11:DG:H5'	2.27	0.49
1:H:4:DG:H1'	1:H:5:DT:H5'	1.95	0.49
3:A:155:SER:H	3:A:158:GLN:HE21	1.57	0.49
2:D:8:DT:H5'	7:D:341:HOH:O	2.13	0.48
4:B:87:VAL:CG1	4:B:127:GLU:HB3	2.42	0.48
4:B:81:VAL:HG12	4:B:81:VAL:O	2.12	0.48
4:B:80:ILE:HD12	4:B:218:ILE:CD1	2.40	0.48
3:A:304:LYS:O	3:A:308:GLU:HG3	2.13	0.48
3:A:226:VAL:HG12	3:A:227:VAL:N	2.29	0.48
3:A:46:LEU:HD23	3:A:127:LEU:HG	1.95	0.48
3:A:317:HIS:HA	3:A:320:GLU:OE1	2.13	0.48
3:A:434:TYR:HB3	3:A:436:GLN:OE1	2.13	0.48
2:D:8:DT:H2''	2:D:9:DG:H5'	1.95	0.48
3:A:76:LEU:HA	7:A:1240:HOH:O	2.14	0.48
3:A:68:ASN:OD1	3:A:70:GLU:HG2	2.14	0.47
3:A:146:TRP:NE1	3:A:175:SER:HB3	2.30	0.47
1:H:11:DG:N3	1:H:11:DG:H5'	2.29	0.47
3:A:174:PHE:CD1	3:A:179:ALA:HB2	2.49	0.47
3:A:257:SER:HA	7:A:1039:HOH:O	2.14	0.46
4:B:56:TYR:HB3	4:B:133:ARG:NH2	2.30	0.46
4:B:98:ARG:HA	4:B:207:GLU:HG3	1.97	0.45
3:A:426:ASN:OD1	4:B:195:SER:HB2	2.15	0.45
3:A:271:VAL:HG12	3:A:298:THR:HG22	1.97	0.45
3:A:360:ASP:OD2	3:A:363:LEU:HG	2.16	0.45
3:A:146:TRP:CE2	3:A:175:SER:HB3	2.52	0.45
3:A:73:ILE:HG22	3:A:74:CYS:N	2.32	0.45
3:A:351:GLN:O	3:A:355:HIS:HB2	2.17	0.45
3:A:232:GLN:NE2	7:A:1207:HOH:O	2.40	0.45
2:D:3:DG:H4'	2:D:4:DG:C4	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:DT:H2''	2:D:7:DT:H5''	1.98	0.45
4:B:97:LEU:HD12	4:B:114:ALA:HA	1.99	0.44
4:B:210:THR:HG23	4:B:210:THR:O	2.17	0.44
2:D:6:DT:H2''	2:D:7:DT:C5'	2.47	0.44
4:B:110:ALA:HB1	4:B:152:ARG:HD2	1.99	0.44
4:B:58:PHE:C	4:B:58:PHE:CD1	2.91	0.43
2:D:4:DG:N3	2:D:4:DG:H2'	2.33	0.43
4:B:75:PHE:CZ	4:B:122:LYS:HG3	2.53	0.43
4:B:44:LYS:HD2	4:B:135:PRO:CG	2.49	0.43
4:B:105:VAL:HG21	7:B:289:HOH:O	2.19	0.43
3:A:309:LEU:HD12	3:A:309:LEU:HA	1.87	0.42
3:A:444:PHE:O	3:A:446:VAL:HG23	2.19	0.42
3:A:449:ASP:OD1	3:A:450:ASN:N	2.51	0.42
4:B:87:VAL:HG11	4:B:127:GLU:HB3	2.00	0.42
3:A:494:ILE:HG13	3:A:495:TYR:CD1	2.54	0.42
4:B:48:PRO:O	4:B:215:ILE:HG21	2.19	0.42
3:A:352:ASP:HB3	3:A:363:LEU:HD11	2.01	0.42
3:A:450:ASN:OD1	3:A:452:HIS:HB2	2.20	0.42
3:A:61:ALA:CB	3:A:76:LEU:HB3	2.48	0.42
3:A:426:ASN:CG	4:B:195:SER:HB2	2.40	0.42
3:A:146:TRP:CZ3	3:A:174:PHE:HA	2.55	0.42
4:B:33:SER:C	4:B:35:LEU:H	2.23	0.42
4:B:47:TYR:HB2	4:B:81:VAL:HG13	2.01	0.41
1:G:8:DT:H4'	1:G:9:DG:C2	2.55	0.41
3:A:458:ARG:O	3:A:462:GLU:HG3	2.20	0.41
3:A:253:PHE:CE2	3:A:286:LYS:HB3	2.56	0.41
3:A:348:THR:CG2	3:A:353:LEU:HD13	2.51	0.41
3:A:386:TRP:CH2	3:A:465:ALA:HB2	2.56	0.41
3:A:416:LEU:CD1	3:A:430:ARG:HG2	2.51	0.41
3:A:460:LYS:HE3	3:A:460:LYS:HB2	1.81	0.41
1:H:1:DG:H1'	1:H:2:DG:H5'	2.02	0.41
1:H:4:DG:H8	7:H:280:HOH:O	2.04	0.41
4:B:61:PRO:HB3	4:B:116:LEU:HD23	2.03	0.41
3:A:272:ARG:HH11	3:A:272:ARG:HG3	1.86	0.41
3:A:87:GLN:O	3:A:91:ALA:HB2	2.22	0.40
3:A:396:LYS:HG2	7:B:264:HOH:O	2.21	0.40
3:A:347:SER:HB3	3:A:372:GLN:HE22	1.86	0.40
3:A:428:THR:HG22	4:B:190:VAL:HB	2.04	0.40
3:A:73:ILE:CG2	3:A:74:CYS:N	2.84	0.40
3:A:170:THR:HA	3:A:171:PRO:HD3	1.94	0.40
3:A:487:LEU:N	3:A:487:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:219:PHE:CE1	4:B:223:LYS:HD2	2.57	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)
7:A:1266:HOH:O	7:A:1266:HOH:O[12_555]	1.01	1.19
7:A:1264:HOH:O	7:A:1264:HOH:O[12_555]	1.02	1.18
4:B:130:ASN:ND2	4:B:130:ASN:ND2[12_555]	1.75	0.45

## 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	
3	A	458/460 (100%)	434 (95%)	19 (4%)	5 (1%)	14	13
4	B	214/216 (99%)	191 (89%)	22 (10%)	1 (0%)	29	32
All	All	672/676 (99%)	625 (93%)	41 (6%)	6 (1%)	17	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	69	GLN
3	A	87	GLN
3	A	89	LYS
3	A	70	GLU
4	B	223	LYS
3	A	84	TYR

### 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	
3	A	408/408 (100%)	392 (96%)	16 (4%)	32	40
4	B	189/189 (100%)	181 (96%)	8 (4%)	30	36
All	All	597/597 (100%)	573 (96%)	24 (4%)	31	39

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	71	ARG
3	A	76	LEU
3	A	167	SER
3	A	207	SER
3	A	239	TYR
3	A	283	THR
3	A	309	LEU
3	A	337	GLU
3	A	353	LEU
3	A	359	SER
3	A	362	GLU
3	A	404	SER
3	A	416	LEU
3	A	460	LYS
3	A	467	LEU
3	A	482	ARG
4	B	31	VAL
4	B	41	CYS
4	B	53	THR
4	B	66	GLU
4	B	92	ASN
4	B	97	LEU
4	B	128	ARG
4	B	215	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	87	GLN
3	A	158	GLN
3	A	327	ASN
3	A	331	ASN
3	A	372	GLN
3	A	426	ASN
4	B	10	GLN
4	B	79	ASN
4	B	92	ASN
4	B	149	GLN
4	B	221	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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(Å²)	Q<0.9
1	G	12/13 (92%)	0.23	0	100 100	37, 45, 57, 58	0
1	H	12/13 (92%)	0.21	0	100 100	41, 51, 61, 61	0
2	D	11/12 (91%)	-0.13	1 (9%)	9 14	26, 37, 52, 58	0
3	A	460/460 (100%)	0.14	18 (3%)	39 52	17, 30, 57, 85	0
4	B	216/216 (100%)	0.64	26 (12%)	4 7	21, 52, 73, 78	0
All	All	711/714 (99%)	0.29	45 (6%)	20 29	17, 35, 69, 85	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	404	SER	9.8
3	A	90	GLY	9.4
3	A	88	GLN	8.2
3	A	91	ALA	7.8
3	A	69	GLN	6.3
3	A	89	LYS	6.2
3	A	92	GLY	6.2
3	A	405	GLY	5.9
3	A	403	ALA	5.6
4	B	125	LEU	4.6
4	B	9	GLN	4.5
4	B	122	LYS	4.3
3	A	344	ALA	3.9
4	B	130	ASN	3.6
4	B	211	ALA	3.6
4	B	126	GLN	3.6
3	A	406	LYS	3.5
4	B	196	LYS	3.4
3	A	87	GLN	3.4
4	B	35	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
4	B	77	ASN	3.4
4	B	65	LYS	3.3
3	A	93	ASP	3.2
4	B	131	PRO	3.0
4	B	99	ARG	2.9
4	B	73	ALA	2.7
2	D	8	DT	2.7
3	A	120	ILE	2.6
4	B	220	VAL	2.6
4	B	179	ALA	2.6
4	B	128	ARG	2.6
4	B	219	PHE	2.6
4	B	197	GLY	2.5
4	B	60	ALA	2.4
4	B	59	VAL	2.3
4	B	209	ASN	2.3
3	A	283	THR	2.2
3	A	70	GLU	2.2
4	B	129	LEU	2.2
4	B	75	PHE	2.1
3	A	76	LEU	2.1
4	B	78	VAL	2.1
3	A	297	ILE	2.1
4	B	50	PHE	2.0
4	B	52	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	A	1005	1/1	0.84	0.36	91,91,91,91	0
5	NA	G	1004	1/1	0.85	0.22	48,48,48,48	0
5	NA	H	1003	1/1	0.95	0.06	42,42,42,42	0
5	NA	G	1001	1/1	0.96	0.17	45,45,45,45	0
5	NA	G	1002	1/1	0.97	0.27	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.