



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:18 PM UTC

PDB ID : 1PA6 / pdb_00001pa6
Title : Crystal structure of the OXYTRICHA nova telomere end-binding protein complexed with noncognate ssDNA GGGGTTTTGAGG
Authors : Theobald, D.L.; Schultz, S.C.
Deposited on : 2003-05-13
Resolution : 2.45 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

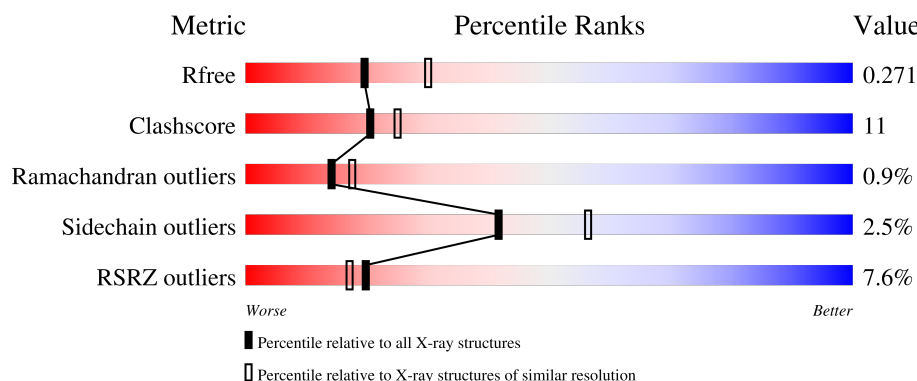
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	D	12	8% 58% 42%
2	G	12	67% 33%
2	H	12	50% 50%
3	A	460	8% 74% 24% .
4	B	216	7% 72% 27% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6705 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*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	12	Total	C	N	O	P	0	0	0
			252	120	48	73	11			

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

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

- 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 (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	2	Total	Na	0	0
			2	2		
5	H	2	Total	Na	0	0
			2	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	36	Total	O	0	0
			36	36		
7	G	35	Total	O	0	0
			35	35		
7	H	35	Total	O	0	0
			35	35		
7	A	329	Total	O	0	0
			329	329		
7	B	68	Total	O	0	0
			68	68		

3 Residue-property plots [i](#)

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 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.

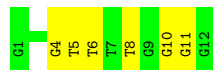
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*AP*GP*G)-3'



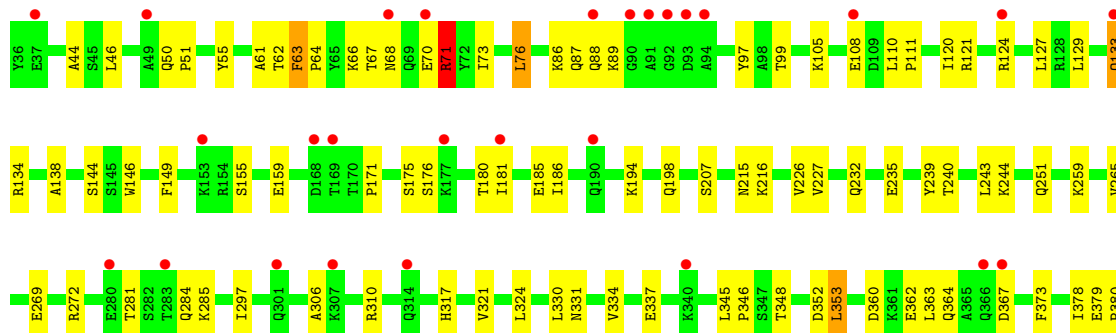
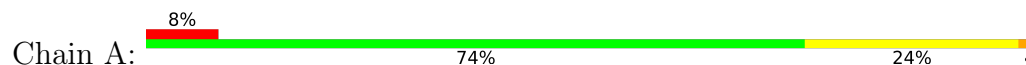
- Molecule 2: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'



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

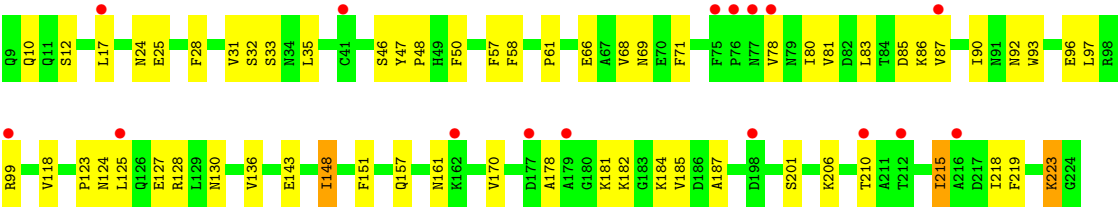


- Molecule 3: Telomere-binding protein alpha subunit





● 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, α , β , γ	93.11Å 93.11Å 422.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.79 – 2.45 29.79 – 2.45	Depositor EDS
% Data completeness (in resolution range)	75.3 (29.79-2.45) 75.3 (29.79-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.268 0.225 , 0.271	Depositor DCC
R_{free} test set	3083 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6705	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

5.1 Standard geometry

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	D	0.51	0/283	0.94	0/438
2	G	0.29	0/284	0.64	0/440
2	H	0.31	0/284	0.65	0/440
3	A	0.52	0/3777	0.99	13/5104 (0.3%)
4	B	0.44	0/1771	0.84	1/2391 (0.0%)
All	All	0.49	0/6399	0.92	14/8813 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	240	THR	N-CA-C	6.91	120.16	108.90
3	A	55	TYR	N-CA-C	-6.27	99.18	109.40
3	A	110	LEU	CA-C-N	6.03	126.23	119.90
3	A	110	LEU	C-N-CA	6.03	126.23	119.90
3	A	476	ASP	N-CA-C	-5.73	99.17	108.52
3	A	62	THR	N-CA-C	-5.60	102.23	110.52
3	A	297	ILE	N-CA-C	5.56	116.12	108.12
3	A	477	ALA	N-CA-C	5.51	117.56	109.24
3	A	63	PHE	N-CA-C	-5.44	102.23	110.39
4	B	148	ILE	N-CA-C	-5.29	105.56	110.53
3	A	71	ARG	N-CA-C	5.28	118.03	109.06
3	A	367	ASP	N-CA-C	-5.16	107.66	114.31
3	A	97	TYR	N-CA-C	5.13	116.33	108.42
3	A	216	LYS	N-CA-C	-5.07	105.80	112.94

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	D	252	0	138	6	0
2	G	253	0	138	3	0
2	H	253	0	138	3	0
3	A	3706	0	3699	78	0
4	B	1733	0	1718	49	1
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	B	1	0	0	1	0
7	A	329	0	0	6	2
7	B	68	0	0	0	0
7	D	36	0	0	2	0
7	G	35	0	0	1	0
7	H	35	0	0	0	0
All	All	6705	0	5831	135	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 11.

All (135) 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)
3:A:99:THR:HG23	3:A:133:GLN:HE22	1.01	1.17
3:A:99:THR:HG23	3:A:133:GLN:NE2	1.81	0.93
3:A:99:THR:CG2	3:A:133:GLN:HE22	1.83	0.92
4:B:80:ILE:HD12	4:B:218:ILE:HD11	1.56	0.86
4:B:10:GLN:HE21	4:B:12:SER:H	1.20	0.86
3:A:345:LEU:HD12	3:A:346:PRO:HD2	1.56	0.85
4:B:96:GLU:OE2	4:B:210:THR:HG22	1.85	0.77
2:H:4:DG:H1'	2:H:5:DT:H5'	1.68	0.74
3:A:272:ARG:HG3	3:A:272:ARG:HH11	1.52	0.73
3:A:281:THR:HB	4:B:10:GLN:HE22	1.53	0.72
1:D:1:DG:H3'	1:D:2:DG:H5''	1.73	0.71
4:B:17:LEU:HD21	4:B:35:LEU:HB3	1.73	0.71
2:G:4:DG:H1'	2:G:5:DT:H5'	1.75	0.69
3:A:66:LYS:HE2	3:A:68:ASN:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:378:ILE:HG21	3:A:386:TRP:CZ2	2.29	0.68
3:A:235:GLU:OE2	3:A:259:LYS:NZ	2.22	0.68
3:A:269:GLU:OE2	7:A:805:HOH:O	2.13	0.67
3:A:324:LEU:HD23	7:A:702:HOH:O	1.95	0.67
4:B:81:VAL:HG11	4:B:219:PHE:HD1	1.58	0.66
3:A:194:LYS:O	3:A:198:GLN:HG3	1.96	0.66
4:B:28:PHE:O	4:B:31:VAL:HG12	1.95	0.65
4:B:87:VAL:HG11	4:B:127:GLU:HB3	1.77	0.65
1:D:10:DA:H3'	7:D:27:HOH:O	1.99	0.63
4:B:71:PHE:CE1	4:B:123:PRO:HD3	2.36	0.61
4:B:81:VAL:HG12	4:B:81:VAL:O	2.01	0.60
3:A:414:GLN:CD	3:A:430:ARG:HD2	2.26	0.60
3:A:306:ALA:O	3:A:310:ARG:HG3	2.01	0.60
4:B:71:PHE:HE1	4:B:123:PRO:HD3	1.67	0.60
4:B:182:LYS:HD2	6:B:605:CL:CL	2.39	0.59
3:A:458:ARG:O	3:A:462:GLU:HG3	2.02	0.58
3:A:284:GLN:HG3	3:A:330:LEU:HD12	1.85	0.57
3:A:373:PHE:CE1	3:A:417:VAL:HG11	2.39	0.57
1:D:1:DG:H3'	1:D:2:DG:C5'	2.34	0.57
3:A:348:THR:CG2	3:A:353:LEU:HD13	2.35	0.57
3:A:352:ASP:HB3	3:A:363:LEU:HD11	1.86	0.57
3:A:155:SER:O	3:A:159:GLU:HG3	2.05	0.57
3:A:215:ASN:HA	3:A:251:GLN:HG3	1.86	0.57
4:B:87:VAL:HG13	4:B:124:ASN:HB2	1.86	0.57
4:B:219:PHE:CE1	4:B:223:LYS:HD2	2.40	0.56
4:B:81:VAL:HG11	4:B:219:PHE:CD1	2.41	0.56
4:B:92:ASN:C	4:B:92:ASN:HD22	2.15	0.54
3:A:285:LYS:HB3	3:A:331:ASN:HD21	1.72	0.54
3:A:402:GLY:O	3:A:403:ALA:HB3	2.09	0.53
3:A:429:TYR:N	3:A:429:TYR:CD1	2.77	0.53
3:A:430:ARG:HD3	7:A:619:HOH:O	2.08	0.53
4:B:17:LEU:CD2	4:B:35:LEU:HB3	2.39	0.52
1:D:12:DG:H2'	1:D:12:DG:N3	2.23	0.52
3:A:404:SER:C	3:A:406:LYS:H	2.19	0.51
3:A:99:THR:CG2	3:A:133:GLN:NE2	2.56	0.51
3:A:272:ARG:HG3	3:A:272:ARG:NH1	2.22	0.51
3:A:215:ASN:CA	3:A:251:GLN:HG3	2.41	0.51
4:B:206:LYS:O	4:B:206:LYS:HG3	2.11	0.51
4:B:148:ILE:O	4:B:151:PHE:HB3	2.12	0.50
3:A:181:ILE:HD12	3:A:181:ILE:N	2.26	0.50
4:B:46:SER:HA	4:B:50:PHE:CD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:378:ILE:HG12	3:A:415:PHE:CD2	2.47	0.49
4:B:92:ASN:HD22	4:B:93:TRP:N	2.10	0.49
3:A:61:ALA:HB2	3:A:76:LEU:HB3	1.95	0.49
4:B:215:ILE:O	4:B:218:ILE:HG22	2.12	0.49
3:A:232:GLN:NE2	3:A:334:VAL:HG23	2.27	0.49
3:A:76:LEU:HD23	3:A:76:LEU:N	2.28	0.48
3:A:111:PRO:HD3	3:A:146:TRP:CE2	2.48	0.48
4:B:24:ASN:C	4:B:25:GLU:HG2	2.39	0.48
4:B:48:PRO:O	4:B:215:ILE:HG21	2.12	0.48
3:A:398:SER:OG	3:A:406:LYS:HB3	2.13	0.48
3:A:405:GLY:O	3:A:406:LYS:HD3	2.14	0.48
3:A:44:ALA:O	3:A:134:ARG:NH2	2.47	0.48
3:A:70:GLU:O	3:A:71:ARG:HD3	2.13	0.48
4:B:57:PHE:CD2	4:B:136:VAL:HG23	2.49	0.48
2:H:10:DG:H2''	2:H:11:DG:C5'	2.44	0.48
3:A:67:THR:HG21	3:A:73:ILE:HD12	1.95	0.47
3:A:149:PHE:CE2	3:A:171:PRO:HG3	2.49	0.47
4:B:47:TYR:CD1	4:B:48:PRO:HA	2.50	0.47
3:A:360:ASP:O	3:A:364:GLN:HG3	2.14	0.47
4:B:99:ARG:NH1	4:B:201:SER:HB2	2.30	0.47
3:A:138:ALA:HB1	3:A:144:SER:HB3	1.97	0.46
3:A:284:GLN:HB2	4:B:143:GLU:OE1	2.16	0.46
4:B:47:TYR:HB2	4:B:81:VAL:HG13	1.98	0.46
4:B:78:VAL:HG21	4:B:125:LEU:HD11	1.99	0.45
4:B:85:ASP:O	4:B:85:ASP:OD1	2.33	0.45
3:A:121:ARG:O	3:A:146:TRP:HA	2.16	0.45
3:A:281:THR:CB	4:B:10:GLN:HE22	2.27	0.45
4:B:58:PHE:C	4:B:58:PHE:CD1	2.95	0.45
4:B:219:PHE:O	4:B:223:LYS:HG2	2.17	0.45
3:A:404:SER:O	3:A:406:LYS:N	2.50	0.45
7:A:539:HOH:O	4:B:184:LYS:HB3	2.16	0.45
3:A:46:LEU:HD23	3:A:127:LEU:HG	1.98	0.44
3:A:175:SER:O	3:A:176:SER:OG	2.19	0.44
1:D:2:DG:H3'	7:D:252:HOH:O	2.16	0.44
1:D:3:DG:N3	1:D:3:DG:H2'	2.33	0.44
3:A:444:PHE:O	3:A:446:VAL:HG23	2.17	0.44
3:A:226:VAL:HG12	3:A:227:VAL:N	2.31	0.44
3:A:414:GLN:OE1	4:B:170:VAL:HG23	2.18	0.44
3:A:127:LEU:HD11	3:A:134:ARG:HB3	1.99	0.44
4:B:78:VAL:CG2	4:B:125:LEU:HD11	2.48	0.44
4:B:32:SER:HB2	4:B:35:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:378:ILE:HG12	3:A:415:PHE:HD2	1.83	0.43
4:B:83:LEU:O	4:B:86:LYS:HB2	2.18	0.43
4:B:50:PHE:O	4:B:61:PRO:HD2	2.17	0.43
3:A:317:HIS:O	3:A:321:VAL:HG23	2.19	0.43
4:B:87:VAL:CG1	4:B:127:GLU:HB3	2.45	0.43
3:A:180:THR:C	3:A:181:ILE:HD12	2.43	0.43
3:A:414:GLN:NE2	7:A:619:HOH:O	2.51	0.43
3:A:149:PHE:CZ	3:A:171:PRO:HG3	2.53	0.43
4:B:33:SER:C	4:B:35:LEU:H	2.27	0.43
2:G:10:DG:H5''	7:G:489:HOH:O	2.19	0.42
3:A:120:ILE:O	3:A:120:ILE:HG23	2.19	0.42
4:B:128:ARG:HA	4:B:128:ARG:HD2	1.60	0.42
3:A:418:LYS:NZ	3:A:427:ASN:O	2.50	0.42
3:A:232:GLN:HB3	3:A:244:LYS:HB3	2.01	0.42
3:A:86:LYS:O	3:A:88:GLN:N	2.52	0.42
4:B:90:ILE:HG23	4:B:118:VAL:HG13	2.01	0.42
3:A:435:THR:HG22	3:A:439:LEU:O	2.20	0.42
3:A:71:ARG:HH11	3:A:105:LYS:HG2	1.84	0.42
3:A:414:GLN:OE1	3:A:430:ARG:HD2	2.20	0.41
4:B:185:VAL:C	4:B:187:ALA:H	2.29	0.41
3:A:402:GLY:O	3:A:403:ALA:CB	2.68	0.41
3:A:185:GLU:O	3:A:186:ILE:C	2.62	0.41
3:A:243:LEU:HD21	3:A:265:VAL:HG11	2.01	0.41
3:A:467:LEU:HD13	7:A:706:HOH:O	2.21	0.41
2:H:6:DT:H2''	2:H:8:DT:O4	2.20	0.41
3:A:348:THR:HG22	3:A:353:LEU:HD13	2.03	0.41
3:A:379:GLU:HA	3:A:380:PRO:C	2.45	0.41
2:G:10:DG:H2''	2:G:11:DG:C5'	2.51	0.41
3:A:243:LEU:N	3:A:243:LEU:CD1	2.83	0.41
3:A:432:LEU:O	3:A:487:LEU:HA	2.21	0.41
4:B:157:GLN:O	4:B:161:ASN:ND2	2.50	0.41
4:B:185:VAL:C	4:B:187:ALA:N	2.79	0.41
3:A:63:PHE:CD2	3:A:64:PRO:HD2	2.56	0.41
3:A:146:TRP:NE1	3:A:175:SER:HB3	2.36	0.41
4:B:178:ALA:HA	4:B:181:LYS:HD2	2.03	0.40
3:A:422:THR:HB	3:A:425:ASN:HD21	1.85	0.40
3:A:51:PRO:HB3	3:A:124:ARG:HA	2.03	0.40
3:A:389:GLY:HA3	3:A:406:LYS:HB2	2.03	0.40
4:B:68:VAL:HG23	4:B:69:ASN:N	2.37	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:748:HOH:O	7:A:748:HOH:O[12_555]	1.76	0.44
4:B:130:ASN:ND2	4:B:130:ASN:ND2[12_555]	2.14	0.06
7:A:524:HOH:O	7:A:524:HOH:O[12_555]	2.15	0.05

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%)	437 (95%)	16 (4%)	5 (1%)	11	12
4	B	214/216 (99%)	194 (91%)	19 (9%)	1 (0%)	24	32
All	All	672/676 (99%)	631 (94%)	35 (5%)	6 (1%)	14	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	87	GLN
3	A	403	ALA
3	A	89	LYS
3	A	404	SER
3	A	405	GLY
4	B	223	LYS

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	
3	A	408/408 (100%)	396 (97%)	12 (3%)	37	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	189/189 (100%)	186 (98%)	3 (2%)	55	69
All	All	597/597 (100%)	582 (98%)	15 (2%)	42	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	50	GLN
3	A	71	ARG
3	A	76	LEU
3	A	108	GLU
3	A	129	LEU
3	A	133	GLN
3	A	207	SER
3	A	239	TYR
3	A	337	GLU
3	A	353	LEU
3	A	362	GLU
3	A	467	LEU
4	B	66	GLU
4	B	97	LEU
4	B	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	87	GLN
3	A	133	GLN
3	A	158	GLN
3	A	178	HIS
3	A	198	GLN
3	A	232	GLN
3	A	241	ASN
3	A	251	GLN
3	A	284	GLN
3	A	327	ASN
3	A	351	GLN
3	A	356	HIS
3	A	412	GLN
3	A	423	GLN
3	A	427	ASN
3	A	442	ASN

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Mol	Chain	Res	Type
4	B	10	GLN
4	B	49	HIS
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 oligosaccharides 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 [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	D	12/12 (100%)	1.11	1 (8%) 17 15	12, 19, 45, 54	9 (75%)
2	G	12/12 (100%)	-0.32	0 100 100	38, 55, 66, 66	0
2	H	12/12 (100%)	-0.02	0 100 100	49, 62, 67, 71	0
3	A	460/460 (100%)	0.19	37 (8%) 18 16	16, 40, 68, 102	21 (4%)
4	B	216/216 (100%)	0.63	16 (7%) 20 18	19, 56, 87, 97	10 (4%)
All	All	712/712 (100%)	0.32	54 (7%) 20 17	12, 43, 82, 102	40 (5%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	76	PRO	10.6
4	B	75	PHE	7.1
4	B	17	LEU	6.9
3	A	169	THR	6.9
4	B	198	ASP	6.9
4	B	78	VAL	6.6
1	D	7	DT	6.3
4	B	77	ASN	6.0
4	B	177	ASP	6.0
3	A	177	LYS	6.0
3	A	466	GLU	6.0
3	A	492	LYS	5.7
3	A	403	ALA	5.5
3	A	301	GLN	5.5
3	A	168	ASP	5.4
4	B	99	ARG	5.4
3	A	133	GLN	5.1
3	A	190	GLN	5.0
3	A	314	GLN	5.0
4	B	162	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
3	A	91	ALA	4.6
3	A	124	ARG	4.6
3	A	92	GLY	4.5
3	A	405	GLY	4.5
3	A	37	GLU	4.3
3	A	460	LYS	4.3
3	A	153	LYS	4.2
3	A	108	GLU	4.1
3	A	447	LYS	4.0
3	A	367	ASP	3.9
3	A	280	GLU	3.6
3	A	307	LYS	3.5
3	A	459	LYS	3.5
3	A	88	GLN	3.2
3	A	340	LYS	3.2
3	A	406	LYS	3.2
4	B	179	ALA	3.0
3	A	90	GLY	3.0
3	A	404	SER	2.9
4	B	125	LEU	2.9
3	A	366	GLN	2.9
3	A	70	GLU	2.8
4	B	87	VAL	2.7
3	A	402	GLY	2.5
3	A	93	ASP	2.5
4	B	212	THR	2.3
3	A	283	THR	2.3
3	A	68	ASN	2.2
4	B	41	CYS	2.2
4	B	210	THR	2.2
3	A	94	ALA	2.2
4	B	216	ALA	2.1
3	A	49	ALA	2.1
3	A	181	ILE	2.1

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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
5	NA	H	602	1/1	0.81	0.20	100,100,100,100	0
5	NA	G	603	1/1	0.84	0.09	63,63,63,63	0
5	NA	H	604	1/1	0.93	0.08	65,65,65,65	0
6	CL	B	605	1/1	0.96	0.08	64,64,64,64	0
5	NA	G	601	1/1	0.98	0.07	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.