



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 AM UTC

PDB ID : 1PHJ / pdb_00001phj
Title : CRYSTAL STRUCTURE OF THE OXYTRICHA NOVA TELOMERE
END-BINDING PROTEIN COMPLEXED WITH NONCOGNATE SSDNA
GG(3DR)GTTTTGGGG
Authors : Theobald, D.L.; Schultz, S.C.
Deposited on : 2003-05-29
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

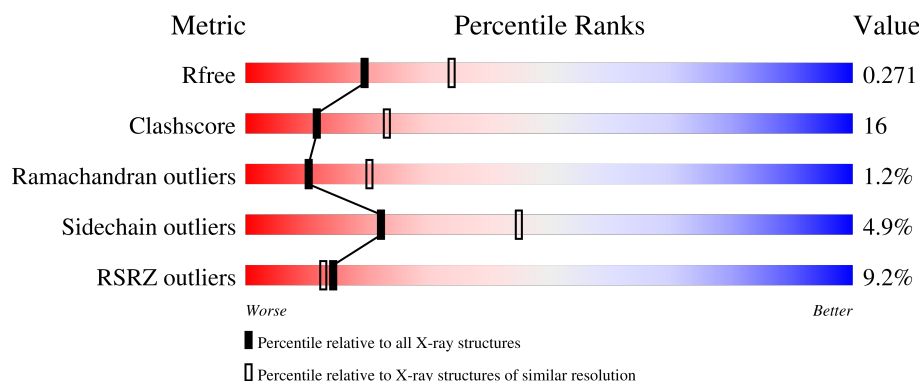
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	G	13	
1	H	13	
2	D	12	
3	A	461	
4	B	216	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6410 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*(3DR)P*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			242	115	43	73	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	449	Total	C	N	O	S	0	0	0
			3636	2312	625	697	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1723	1107	292	323	1			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	5	Total	O	0	0
			5	5		
5	D	18	Total	O	0	0
			18	18		

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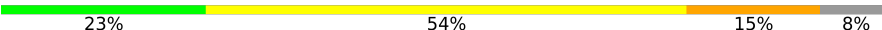
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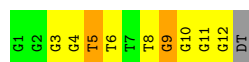
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	5	Total 5	O 5	0	0
5	A	232	Total 232	O 232	0	0
5	B	43	Total 43	O 43	0	0

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.

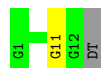
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*GP*T)-3'

Chain G: 



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

Chain H: 



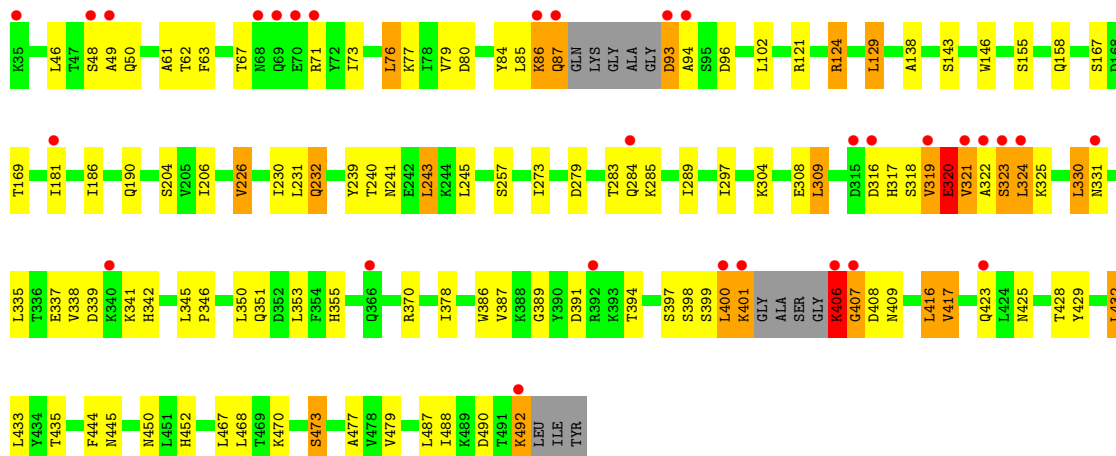
- Molecule 2: 5'-D(*GP*GP*(3DR)P*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain D: 

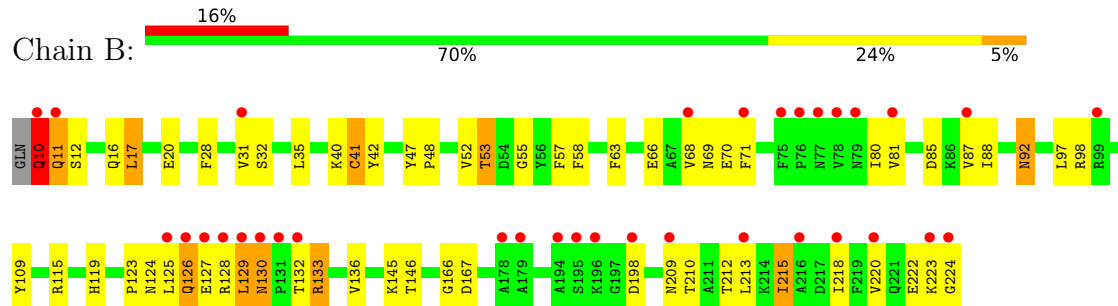


- Molecule 3: Telomere-binding protein alpha subunit

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, α , β , γ	93.48Å 93.48Å 423.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.31 – 2.50 27.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (27.31-2.50) 92.8 (27.31-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.273 0.245 , 0.271	Depositor DCC
R_{free} test set	4755 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.8	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	0.90	EDS
Total number of atoms	6410	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: 3DR

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	0.36	0/284	0.98	4/440 (0.9%)
1	H	0.28	0/284	0.67	0/440
2	D	0.30	0/258	0.72	0/397
3	A	0.78	23/3706 (0.6%)	1.11	34/5010 (0.7%)
4	B	1.00	5/1761 (0.3%)	0.98	8/2379 (0.3%)
All	All	0.81	28/6293 (0.4%)	1.04	46/8666 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	B	0	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	10	GLN	N-CA	28.56	2.00	1.46
4	B	10	GLN	CA-C	21.84	1.98	1.52
3	A	401	LYS	CA-C	13.11	1.69	1.52
3	A	406	LYS	CA-C	12.98	1.70	1.52
3	A	492	LYS	CA-C	12.62	1.79	1.52
4	B	11	GLN	N-CA	12.42	1.62	1.46
3	A	323	SER	CA-C	-12.29	1.35	1.52
3	A	406	LYS	N-CA	10.94	1.60	1.46
4	B	11	GLN	CA-C	8.73	1.62	1.52
3	A	401	LYS	CB-CG	8.71	1.78	1.52
3	A	407	GLY	N-CA	8.06	1.54	1.45
3	A	407	GLY	CA-C	7.96	1.61	1.52
3	A	324	LEU	N-CA	-7.81	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	320	GLU	N-CA	-7.75	1.36	1.46
3	A	320	GLU	CA-C	7.34	1.62	1.52
3	A	319	VAL	CA-C	-7.21	1.41	1.52
3	A	401	LYS	CA-CB	7.09	1.64	1.53
3	A	492	LYS	N-CA	6.86	1.59	1.46
3	A	401	LYS	N-CA	-6.76	1.38	1.46
3	A	401	LYS	CG-CD	6.75	1.72	1.52
3	A	406	LYS	C-N	6.72	1.39	1.33
4	B	10	GLN	CB-CG	6.43	1.71	1.52
3	A	87	GLN	CA-C	6.24	1.60	1.52
3	A	400	LEU	CA-C	-6.08	1.46	1.53
3	A	408	ASP	N-CA	5.88	1.53	1.46
3	A	401	LYS	C-N	5.73	1.41	1.33
3	A	323	SER	N-CA	5.44	1.53	1.46
3	A	401	LYS	CD-CE	5.09	1.67	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	LYS	N-CA-C	-18.61	86.70	112.94
4	B	10	GLN	N-CA-C	16.14	156.18	111.00
3	A	86	LYS	N-CA-C	-15.87	88.45	110.35
4	B	10	GLN	CB-CA-C	-13.67	84.13	110.10
3	A	407	GLY	N-CA-C	13.61	129.38	110.74
3	A	406	LYS	N-CA-C	12.43	137.28	110.80
3	A	408	ASP	N-CA-C	-10.86	91.44	109.46
3	A	401	LYS	CB-CA-C	9.97	127.79	110.64
3	A	87	GLN	CA-C-N	9.46	139.60	121.54
3	A	87	GLN	C-N-CA	9.46	139.60	121.54
3	A	87	GLN	CB-CA-C	8.38	125.77	111.68
3	A	94	ALA	N-CA-C	-7.62	101.04	110.41
4	B	11	GLN	N-CA-C	7.23	122.55	113.43
3	A	492	LYS	CA-C-O	-7.14	108.66	120.80
1	G	5	DT	C5'-C4'-C3'	-6.83	104.66	114.90
4	B	10	GLN	CA-C-N	6.77	136.59	122.58
4	B	10	GLN	C-N-CA	6.77	136.59	122.58
3	A	400	LEU	CA-CB-CG	-6.73	92.74	116.30
3	A	401	LYS	CB-CG-CD	6.57	126.40	111.30
3	A	323	SER	N-CA-CB	6.43	119.98	110.33
3	A	297	ILE	N-CA-C	6.17	116.75	108.11
3	A	409	ASN	N-CA-C	5.99	119.29	109.76
3	A	323	SER	CA-CB-OG	5.97	123.05	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	320	GLU	N-CA-C	-5.90	98.24	110.80
3	A	87	GLN	CB-CG-CD	5.82	122.50	112.60
1	G	9	DG	C5'-C4'-C3'	5.78	123.56	114.90
3	A	63	PHE	N-CA-C	-5.74	102.37	110.29
3	A	319	VAL	CA-C-N	-5.74	110.58	121.54
3	A	319	VAL	C-N-CA	-5.74	110.58	121.54
3	A	240	THR	N-CA-C	5.68	118.72	109.24
3	A	417	VAL	N-CA-C	5.59	116.90	108.96
3	A	93	ASP	N-CA-C	5.58	122.68	110.80
3	A	428	THR	N-CA-C	-5.56	99.61	109.06
3	A	62	THR	N-CA-C	-5.55	103.37	110.53
1	G	10	DG	C5'-C4'-C3'	5.48	123.11	114.90
1	G	9	DG	C4'-C3'-O3'	-5.47	101.80	110.00
4	B	10	GLN	O-C-N	-5.46	114.27	123.00
4	B	11	GLN	CB-CA-C	-5.41	100.56	109.65
3	A	93	ASP	N-CA-CB	5.32	119.48	110.49
3	A	477	ALA	N-CA-C	5.23	117.14	109.24
3	A	432	LEU	N-CA-C	5.21	118.56	110.17
3	A	319	VAL	N-CA-C	-5.20	104.41	111.89
4	B	133	ARG	N-CA-C	-5.18	104.03	110.41
3	A	435	THR	N-CA-C	5.14	119.19	113.02
3	A	86	LYS	CA-C-N	-5.00	114.33	122.34
3	A	86	LYS	C-N-CA	-5.00	114.33	122.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	10	GLN	Mainchain

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	G	253	0	138	12	0
1	H	253	0	138	1	0
2	D	242	0	135	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3636	0	3633	93	0
4	B	1723	0	1710	78	0
5	A	232	0	0	4	0
5	B	43	0	0	0	0
5	D	18	0	0	1	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0
All	All	6410	0	5754	188	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 16.

All (188) 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:401:LYS:CB	3:A:401:LYS:CG	1.78	1.56
3:A:492:LYS:CA	3:A:492:LYS:C	1.79	1.55
4:B:10:GLN:CA	4:B:10:GLN:C	1.98	1.35
4:B:10:GLN:CA	4:B:10:GLN:N	2.00	1.24
1:G:5:DT:H2''	1:G:6:DT:H5''	1.20	1.10
4:B:80:ILE:HD12	4:B:218:ILE:HD11	1.42	1.01
2:D:6:DT:H2''	2:D:7:DT:H5'	1.51	0.93
3:A:285:LYS:HB3	3:A:331:ASN:HD21	1.33	0.93
4:B:10:GLN:C	4:B:10:GLN:CB	2.42	0.92
1:G:4:DG:H2''	1:G:5:DT:H5''	1.52	0.90
4:B:40:LYS:HD3	4:B:128:ARG:NH2	1.93	0.84
4:B:10:GLN:N	4:B:10:GLN:HA	1.91	0.83
1:G:4:DG:C2'	1:G:5:DT:H5''	2.11	0.80
3:A:226:VAL:HG13	3:A:273:ILE:HB	1.65	0.79
4:B:10:GLN:HE21	4:B:12:SER:H	1.28	0.78
4:B:126:GLN:HE21	4:B:128:ARG:HD3	1.49	0.78
4:B:132:THR:HG22	4:B:133:ARG:O	1.87	0.74
3:A:320:GLU:O	3:A:322:ALA:N	2.22	0.73
2:D:12:DG:H2'	2:D:12:DG:N3	2.06	0.70
3:A:67:THR:HG21	3:A:73:ILE:HD12	1.75	0.68
3:A:285:LYS:HB3	3:A:331:ASN:ND2	2.09	0.67
3:A:76:LEU:HD23	3:A:76:LEU:N	2.10	0.67
4:B:129:LEU:O	4:B:130:ASN:HB2	1.97	0.65
3:A:285:LYS:CB	3:A:331:ASN:HD21	2.09	0.65
4:B:215:ILE:O	4:B:218:ILE:HG22	1.96	0.65
3:A:319:VAL:O	3:A:319:VAL:HG12	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:17:LEU:HD11	4:B:35:LEU:HB3	1.79	0.63
4:B:126:GLN:HG3	4:B:128:ARG:HG2	1.80	0.63
4:B:10:GLN:NE2	4:B:12:SER:H	1.96	0.63
4:B:68:VAL:HG21	4:B:213:LEU:HD11	1.80	0.63
3:A:492:LYS:C	3:A:492:LYS:HA	2.14	0.63
1:G:5:DT:C2'	1:G:6:DT:H5''	2.13	0.62
4:B:28:PHE:O	4:B:31:VAL:HG12	1.99	0.62
4:B:40:LYS:HD3	4:B:128:ARG:HH21	1.65	0.62
3:A:61:ALA:HB2	3:A:76:LEU:HB3	1.81	0.61
1:H:11:DG:H5'	1:H:11:DG:N3	2.15	0.61
4:B:20:GLU:HB3	4:B:31:VAL:HG23	1.81	0.61
4:B:47:TYR:CG	4:B:48:PRO:HA	2.35	0.61
3:A:389:GLY:HA3	3:A:407:GLY:HA3	1.83	0.61
4:B:125:LEU:HD12	4:B:125:LEU:H	1.65	0.60
3:A:401:LYS:O	5:A:708:HOH:O	2.16	0.60
3:A:423:GLN:HG3	5:A:705:HOH:O	2.02	0.60
4:B:10:GLN:HE21	4:B:12:SER:N	1.96	0.58
1:G:4:DG:H2''	1:G:5:DT:C5'	2.30	0.58
3:A:169:THR:OG1	3:A:181:ILE:HD13	2.04	0.58
4:B:87:VAL:CG1	4:B:128:ARG:HG3	2.33	0.58
3:A:79:VAL:HG13	3:A:84:TYR:HB3	1.86	0.58
3:A:86:LYS:N	3:A:96:ASP:HB2	2.19	0.57
4:B:10:GLN:NE2	4:B:11:GLN:H	2.02	0.57
3:A:492:LYS:CA	3:A:492:LYS:O	2.46	0.57
4:B:109:TYR:CE1	4:B:145:LYS:HE2	2.39	0.57
3:A:155:SER:H	3:A:158:GLN:NE2	2.02	0.57
1:G:11:DG:H1'	1:G:12:DG:H5'	1.86	0.57
4:B:47:TYR:CD1	4:B:48:PRO:HA	2.40	0.57
3:A:124:ARG:HG3	3:A:124:ARG:NH1	2.20	0.56
4:B:48:PRO:O	4:B:215:ILE:HG21	2.05	0.56
4:B:87:VAL:HG11	4:B:128:ARG:HG3	1.88	0.56
3:A:391:ASP:HB3	3:A:394:THR:HG22	1.89	0.54
3:A:48:SER:C	3:A:50:GLN:H	2.15	0.54
3:A:124:ARG:HG3	3:A:124:ARG:HH11	1.73	0.54
4:B:132:THR:HG22	4:B:133:ARG:N	2.23	0.54
4:B:132:THR:CG2	4:B:133:ARG:N	2.71	0.54
4:B:126:GLN:NE2	4:B:128:ARG:HD3	2.21	0.54
3:A:317:HIS:HA	3:A:320:GLU:OE1	2.08	0.54
4:B:57:PHE:CD2	4:B:136:VAL:HG23	2.43	0.54
3:A:401:LYS:O	3:A:406:LYS:HB2	2.08	0.54
3:A:79:VAL:CG1	3:A:80:ASP:N	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:126:GLN:O	4:B:127:GLU:C	2.52	0.53
3:A:391:ASP:CG	3:A:394:THR:HG22	2.34	0.53
3:A:230:ILE:HD12	3:A:243:LEU:HG	1.91	0.53
2:D:10:DG:N3	2:D:10:DG:H2'	2.24	0.52
3:A:323:SER:C	3:A:325:LYS:H	2.16	0.52
3:A:432:LEU:HB2	3:A:487:LEU:HD22	1.91	0.52
4:B:129:LEU:O	4:B:130:ASN:CB	2.58	0.52
1:G:4:DG:H1'	1:G:5:DT:H5''	1.91	0.52
3:A:323:SER:C	3:A:325:LYS:N	2.63	0.52
4:B:47:TYR:HB2	4:B:81:VAL:CG1	2.39	0.52
4:B:87:VAL:HG13	4:B:124:ASN:HB2	1.91	0.52
4:B:126:GLN:HE21	4:B:128:ARG:CD	2.21	0.52
1:G:6:DT:H2''	1:G:8:DT:O4	2.09	0.52
4:B:17:LEU:CD1	4:B:35:LEU:HB3	2.39	0.52
3:A:85:LEU:C	3:A:86:LYS:O	2.47	0.52
3:A:46:LEU:CD2	3:A:129:LEU:HD13	2.41	0.51
4:B:55:GLY:HA2	4:B:132:THR:HG21	1.93	0.51
2:D:4:DG:H3'	2:D:4:DG:OP2	2.10	0.51
3:A:230:ILE:HD13	3:A:245:LEU:CD2	2.41	0.51
1:G:4:DG:C1'	1:G:5:DT:H5''	2.40	0.51
4:B:212:THR:HG22	4:B:213:LEU:N	2.25	0.51
3:A:85:LEU:C	3:A:96:ASP:HB2	2.35	0.51
1:G:3:DG:H2'	1:G:3:DG:N3	2.26	0.51
3:A:241:ASN:HB2	3:A:257:SER:O	2.11	0.50
3:A:285:LYS:HD3	3:A:331:ASN:ND2	2.26	0.50
3:A:71:ARG:NE	3:A:73:ILE:HD11	2.25	0.50
4:B:71:PHE:HE1	4:B:123:PRO:HG3	1.77	0.50
3:A:283:THR:HG21	4:B:10:GLN:N	2.26	0.50
3:A:79:VAL:CG1	3:A:84:TYR:HB3	2.41	0.50
3:A:399:SER:C	3:A:401:LYS:H	2.20	0.50
3:A:230:ILE:HD13	3:A:245:LEU:HD23	1.94	0.50
3:A:124:ARG:HH11	3:A:124:ARG:CG	2.25	0.49
3:A:319:VAL:O	3:A:319:VAL:CG1	2.57	0.49
1:G:9:DG:H2'	1:G:9:DG:N3	2.28	0.49
4:B:92:ASN:HB3	4:B:119:HIS:HB2	1.95	0.49
4:B:10:GLN:C	4:B:10:GLN:HB3	2.34	0.48
4:B:81:VAL:HG23	4:B:222:GLU:OE1	2.13	0.48
4:B:220:VAL:HG13	4:B:224:GLY:HA2	1.96	0.48
4:B:42:TYR:CE1	4:B:85:ASP:HA	2.48	0.48
4:B:212:THR:CG2	4:B:213:LEU:N	2.76	0.48
3:A:76:LEU:N	3:A:76:LEU:CD2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:345:LEU:HD23	3:A:370:ARG:HB2	1.96	0.48
4:B:47:TYR:HB2	4:B:81:VAL:HG13	1.96	0.47
3:A:330:LEU:HD22	4:B:146:THR:HG22	1.97	0.47
3:A:350:LEU:HD21	3:A:417:VAL:HG23	1.95	0.47
3:A:80:ASP:C	3:A:80:ASP:OD1	2.57	0.47
3:A:339:ASP:OD1	3:A:341:LYS:HG2	2.15	0.47
3:A:387:VAL:HG12	3:A:400:LEU:HD12	1.96	0.47
4:B:58:PHE:C	4:B:58:PHE:CD1	2.93	0.47
4:B:87:VAL:CG1	4:B:124:ASN:HB2	2.45	0.47
3:A:79:VAL:HG12	3:A:80:ASP:N	2.29	0.47
2:D:6:DT:H2''	2:D:7:DT:C5'	2.36	0.47
4:B:126:GLN:HG3	4:B:128:ARG:HD3	1.97	0.46
4:B:223:LYS:O	4:B:224:GLY:C	2.57	0.46
3:A:429:TYR:N	3:A:429:TYR:CD1	2.83	0.46
3:A:338:VAL:CG1	3:A:342:HIS:HB2	2.46	0.46
3:A:309:LEU:HD12	3:A:309:LEU:HA	1.75	0.45
4:B:126:GLN:HG3	4:B:128:ARG:CG	2.44	0.45
3:A:378:ILE:HG21	3:A:386:TRP:CZ2	2.52	0.45
3:A:391:ASP:HB3	3:A:394:THR:CG2	2.46	0.45
2:D:8:DT:H2''	2:D:9:DG:H5'	1.98	0.45
4:B:127:GLU:O	4:B:129:LEU:HG	2.17	0.45
4:B:10:GLN:C	4:B:10:GLN:CG	2.89	0.44
4:B:125:LEU:O	4:B:127:GLU:N	2.50	0.44
3:A:186:ILE:O	3:A:190:GLN:HG2	2.18	0.44
3:A:318:SER:C	3:A:320:GLU:N	2.72	0.44
4:B:81:VAL:HG12	4:B:81:VAL:O	2.17	0.44
3:A:335:LEU:CD1	3:A:468:LEU:HD23	2.48	0.44
3:A:444:PHE:O	3:A:445:ASN:HB2	2.18	0.44
4:B:109:TYR:CE2	4:B:145:LYS:HG2	2.53	0.43
1:G:11:DG:H2''	1:G:12:DG:C8	2.53	0.43
3:A:416:LEU:HA	3:A:416:LEU:HD12	1.78	0.43
3:A:155:SER:H	3:A:158:GLN:HE21	1.65	0.43
3:A:433:LEU:HD12	3:A:488:ILE:HB	2.00	0.43
3:A:479:VAL:HG12	3:A:488:ILE:HD13	2.00	0.43
4:B:41:CYS:HB3	4:B:53:THR:O	2.19	0.43
3:A:121:ARG:O	3:A:146:TRP:HA	2.19	0.43
3:A:167:SER:OG	3:A:169:THR:HG22	2.19	0.43
4:B:68:VAL:HG11	4:B:213:LEU:HD12	2.00	0.43
4:B:98:ARG:HG3	4:B:115:ARG:HD2	1.99	0.43
4:B:166:GLY:O	4:B:167:ASP:C	2.62	0.43
3:A:71:ARG:CZ	3:A:73:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:68:VAL:HG11	4:B:218:ILE:HD12	2.01	0.42
4:B:97:LEU:C	4:B:98:ARG:HG2	2.43	0.42
4:B:209:ASN:OD1	4:B:209:ASN:N	2.47	0.42
3:A:204:SER:O	3:A:206:ILE:N	2.52	0.42
3:A:401:LYS:CA	5:A:708:HOH:O	2.68	0.42
3:A:320:GLU:O	3:A:321:VAL:C	2.62	0.42
3:A:338:VAL:CG1	3:A:339:ASP:N	2.83	0.42
4:B:52:VAL:HG11	4:B:88:ILE:HD11	2.00	0.42
3:A:391:ASP:CB	3:A:394:THR:HG22	2.48	0.42
3:A:450:ASN:OD1	3:A:452:HIS:HB2	2.20	0.42
3:A:351:GLN:O	3:A:355:HIS:HB2	2.20	0.42
3:A:304:LYS:HE2	3:A:308:GLU:OE2	2.19	0.41
3:A:284:GLN:HG3	3:A:330:LEU:HG	2.01	0.41
3:A:389:GLY:O	3:A:397:SER:HA	2.19	0.41
3:A:425:ASN:HA	4:B:198:ASP:O	2.20	0.41
5:D:158:HOH:O	3:A:77:LYS:HE3	2.19	0.41
3:A:335:LEU:HD12	3:A:468:LEU:HD23	2.02	0.41
3:A:339:ASP:HB2	3:A:490:ASP:HB3	2.03	0.41
3:A:46:LEU:HD22	3:A:129:LEU:HD13	2.02	0.41
3:A:400:LEU:HD23	3:A:406:LYS:H	1.85	0.41
3:A:470:LYS:O	3:A:473:SER:HB2	2.21	0.41
2:D:7:DT:H6	2:D:7:DT:H2'	1.70	0.41
3:A:279:ASP:HB2	3:A:289:ILE:HG13	2.02	0.41
4:B:85:ASP:O	4:B:85:ASP:OD1	2.38	0.41
3:A:71:ARG:NH2	3:A:73:ILE:HD11	2.36	0.41
3:A:124:ARG:NH1	3:A:143:SER:O	2.53	0.41
4:B:55:GLY:O	4:B:132:THR:HG23	2.20	0.41
4:B:126:GLN:H	4:B:126:GLN:HG2	1.71	0.41
3:A:71:ARG:HE	3:A:73:ILE:HD11	1.85	0.41
3:A:102:LEU:HD23	3:A:138:ALA:HB3	2.02	0.41
3:A:232:GLN:NE2	5:A:726:HOH:O	2.27	0.40
4:B:31:VAL:O	4:B:32:SER:C	2.64	0.40
4:B:87:VAL:HG22	4:B:88:ILE:N	2.36	0.40
4:B:127:GLU:O	4:B:127:GLU:HG3	2.21	0.40
3:A:345:LEU:HD12	3:A:346:PRO:HD2	2.03	0.40
4:B:53:THR:HA	4:B:57:PHE:O	2.21	0.40
4:B:10:GLN:HG2	4:B:16:GLN:HB2	2.03	0.40
4:B:63:PHE:O	4:B:212:THR:HG23	2.21	0.40
4:B:68:VAL:HG23	4:B:69:ASN:N	2.36	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	
3	A	447/461 (97%)	421 (94%)	21 (5%)	5 (1%)	11	22
4	B	213/216 (99%)	189 (89%)	21 (10%)	3 (1%)	9	17
All	All	660/677 (98%)	610 (92%)	42 (6%)	8 (1%)	10	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	93	ASP
3	A	321	VAL
3	A	406	LYS
4	B	126	GLN
4	B	130	ASN
4	B	210	THR
3	A	320	GLU
3	A	49	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	
3	A	403/409 (98%)	383 (95%)	20 (5%)	22	44
4	B	188/189 (100%)	179 (95%)	9 (5%)	23	46
All	All	591/598 (99%)	562 (95%)	29 (5%)	22	45

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	76	LEU
3	A	87	GLN
3	A	124	ARG
3	A	129	LEU
3	A	226	VAL
3	A	231	LEU
3	A	232	GLN
3	A	239	TYR
3	A	243	LEU
3	A	309	LEU
3	A	316	ASP
3	A	320	GLU
3	A	324	LEU
3	A	330	LEU
3	A	337	GLU
3	A	353	LEU
3	A	398	SER
3	A	416	LEU
3	A	467	LEU
3	A	473	SER
4	B	10	GLN
4	B	17	LEU
4	B	41	CYS
4	B	53	THR
4	B	66	GLU
4	B	70	GLU
4	B	92	ASN
4	B	129	LEU
4	B	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	158	GLN
3	A	327	ASN
3	A	331	ASN
3	A	372	GLN
3	A	427	ASN
4	B	10	GLN
4	B	11	GLN
4	B	16	GLN
4	B	49	HIS
4	B	92	ASN

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Mol	Chain	Res	Type
4	B	126	GLN
4	B	149	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	3DR	D	3	2	8,11,12	0.28	0	7,14,17	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3DR	D	3	2	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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

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	G	12/13 (92%)	0.71	0	100 100	34, 43, 49, 50	0
1	H	12/13 (92%)	0.68	0	100 100	40, 46, 50, 50	0
2	D	11/12 (91%)	0.23	0	100 100	25, 34, 52, 52	0
3	A	449/461 (97%)	0.29	30 (6%)	24 21	17, 29, 49, 60	0
4	B	215/216 (99%)	1.00	34 (15%)	5 4	23, 46, 61, 70	0
All	All	699/715 (97%)	0.52	64 (9%)	14 13	17, 33, 57, 70	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	407	GLY	8.0
3	A	406	LYS	7.2
4	B	78	VAL	6.3
3	A	319	VAL	6.2
4	B	130	ASN	5.3
3	A	401	LYS	5.2
4	B	129	LEU	4.9
4	B	195	SER	4.7
3	A	87	GLN	4.6
3	A	321	VAL	4.5
3	A	94	ALA	4.5
4	B	127	GLU	4.5
4	B	10	GLN	4.4
4	B	79	ASN	4.3
3	A	93	ASP	4.0
4	B	131	PRO	3.8
3	A	70	GLU	3.6
4	B	179	ALA	3.6
4	B	126	GLN	3.4
4	B	125	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	400	LEU	3.0
4	B	223	LYS	2.9
4	B	87	VAL	2.9
4	B	77	ASN	2.9
4	B	196	LYS	2.9
4	B	218	ILE	2.8
4	B	178	ALA	2.8
3	A	69	GLN	2.8
3	A	423	GLN	2.8
3	A	48	SER	2.7
3	A	324	LEU	2.7
4	B	216	ALA	2.7
3	A	284	GLN	2.7
3	A	86	LYS	2.7
4	B	132	THR	2.7
3	A	315	ASP	2.6
4	B	31	VAL	2.6
4	B	194	ALA	2.6
4	B	198	ASP	2.5
3	A	68	ASN	2.5
4	B	99	ARG	2.5
4	B	213	LEU	2.5
3	A	323	SER	2.4
4	B	76	PRO	2.4
4	B	128	ARG	2.4
4	B	75	PHE	2.4
3	A	316	ASP	2.3
4	B	224	GLY	2.3
3	A	366	GLN	2.3
4	B	11	GLN	2.3
3	A	35	LYS	2.3
3	A	492	LYS	2.3
4	B	220	VAL	2.3
3	A	322	ALA	2.3
3	A	181	ILE	2.3
3	A	331	ASN	2.2
3	A	71	ARG	2.2
3	A	392	ARG	2.2
4	B	71	PHE	2.2
4	B	81	VAL	2.1
4	B	68	VAL	2.1
3	A	340	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	209	ASN	2.1
3	A	49	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	3DR	D	3	11/12	0.74	0.19	50,53,63,68	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.