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Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:49 pm GMT

PDB ID	:	1PHJ
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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	Percentile Ranks	Value
Rfree		0.271
Clashscore		15
Ramachandran outliers		1.2%
Sidechain outliers		4.2%
RSRZ outliers		4.3%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
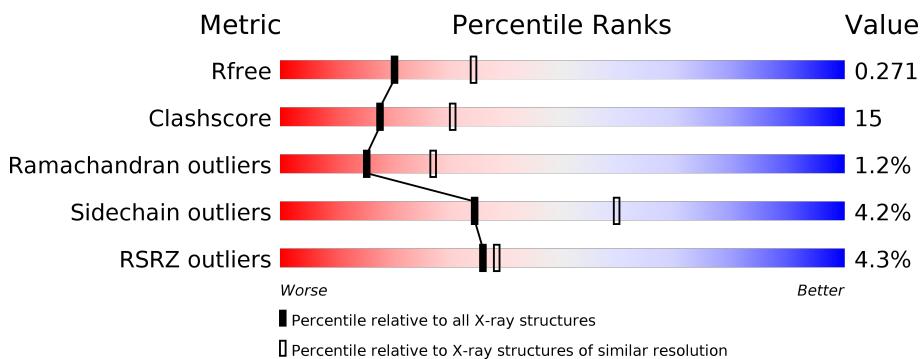
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	23% 54% 15% 8%
1	H	13	85% 8% 8%
2	D	12	33% 67%
3	A	461	2% / 73% 20% · ·
4	B	216	9% / 73% 23% ·
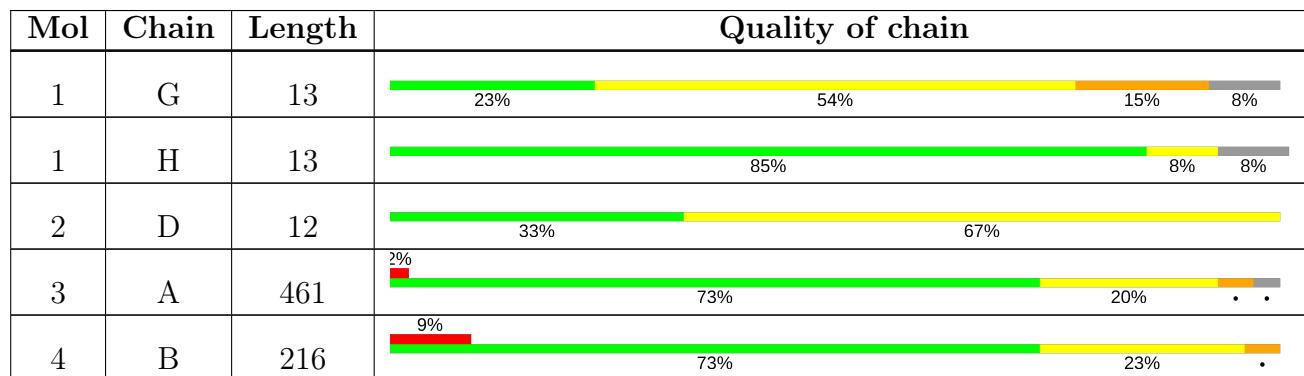
2 Entry composition ⓘ

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 253	C 120	N 48	O 74	P 11	0	0	0
1	H	12	Total 253	C 120	N 48	O 74	P 11	0	0	0

- 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 242	C 115	N 43	O 73	P 11	0	0	0

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

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

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

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

- Molecule 5 is water.

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

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

23% | 54% | 15% | 8%

G1 G2 G3 G4 T5 T6 T7 T8 G9 G10 G11 G12 DT

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

Chain H:

85% | 8% | 8%

G1 G11 G12 DT
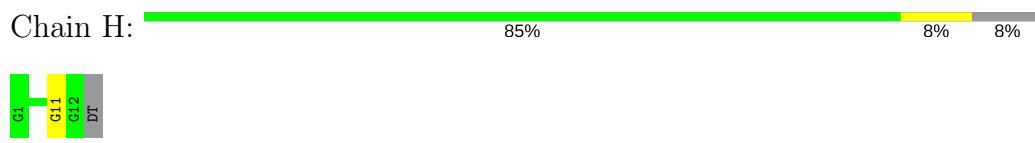
- Molecule 2: 5'-D(*GP*GP*(3DR)P*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain D:

33% | 67%

G1 G4 T5 T6 T7 T8 G9 G10 G11 G12

- Molecule 3: Telomere-binding protein alpha subunit

Chain A:

2% | 73% | 20% | · ·

K35 L46 T47 S48 A49 Q50 A61 T67 N68 Q69 E70 R71 Y72 I73 L76 K77 I78 V79 D80 Y84 L85 K86 Q87 GLN LYS GLY ALA GLY D93 A94 S95 D96 L102 R121 R124 L129 A138 S143 W146 S155 Q158 S167 D168 T169

I181 I186 Q190 S204 V205 I206 V226 I230 L231 Q232 Y239 T240 N241 E242 L243 K244 L245 S257 I273 D279 T283 Q284 K285 I289 K304 E308 L309 D316 H317 S318 V319 E320 V321 A322 S323 L324 K325 L330 N331 L335 T336 E337 V338 D339

K340 K341 H342 L345 P346 L350 Q351 D352 L353 F354 H355 R370 I378 W386 V387 K388 G389 Y390 D391 T394 S397 S398 S399 L400 K401 GLY ALA SER GLY K406 G407 D408 L416 V417 Q423 L424 N425 Y429 L432 L433 F444 N445 N450 L451 H452 L468

T469 K470 F471 N472 S473 V479 L487 I488 K489 D490 T491 K492 LEU ILE TYR

- Molecule 4: Telomere-binding protein beta subunit
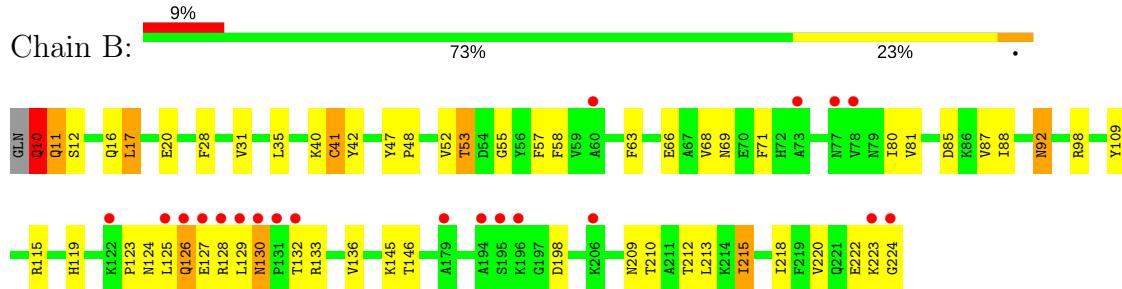
4 Data and refinement statistics ⓘ

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 27.30 – 2.25	Depositor EDS
% Data completeness (in resolution range)	92.9 (27.31-2.50) 90.0 (27.30-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	3594 reflections (9.85%)	DCC
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 , 34.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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	0.57	0/284	1.00	3/440 (0.7%)
1	H	0.32	0/284	0.74	0/440
2	D	0.41	1/258 (0.4%)	0.73	0/397
3	A	0.58	14/3706 (0.4%)	0.79	14/5010 (0.3%)
4	B	0.88	4/1761 (0.2%)	0.72	4/2379 (0.2%)
All	All	0.66	19/6293 (0.3%)	0.78	21/8666 (0.2%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	10	GLN	N-CA	27.08	2.00	1.46
4	B	10	GLN	CA-C	17.64	1.98	1.52
3	A	492	LYS	CA-C	10.19	1.79	1.52
3	A	401	LYS	CB-CG	9.64	1.78	1.52
4	B	11	GLN	N-CA	8.31	1.62	1.46
4	B	10	GLN	CB-CG	7.11	1.71	1.52
3	A	406	LYS	N-CA	6.98	1.60	1.46
3	A	323	SER	CA-C	-6.75	1.35	1.52
3	A	406	LYS	CA-C	6.62	1.70	1.52
3	A	401	LYS	CD-CE	6.59	1.67	1.51
3	A	492	LYS	N-CA	6.46	1.59	1.46
3	A	401	LYS	CA-C	6.38	1.69	1.52
3	A	407	GLY	CA-C	6.13	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	LYS	CG-CD	5.96	1.72	1.52
3	A	407	GLY	N-CA	5.54	1.54	1.46
3	A	87	GLN	CB-CG	5.38	1.67	1.52
3	A	324	LEU	N-CA	-5.12	1.36	1.46
3	A	320	GLU	N-CA	-5.08	1.36	1.46
2	D	1	DG	C4'-C3'	-5.04	1.47	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	10	GLN	N-CA-C	16.73	156.18	111.00
4	B	10	GLN	CB-CA-C	-13.14	84.13	110.40
3	A	400	LEU	CA-CB-CG	-9.81	92.74	115.30
3	A	406	LYS	N-CA-C	9.73	137.28	111.00
3	A	401	LYS	N-CA-C	-9.00	86.70	111.00
3	A	401	LYS	CB-CA-C	8.70	127.79	110.40
3	A	86	LYS	N-CA-C	-8.35	88.45	111.00
3	A	87	GLN	CB-CA-C	7.68	125.77	110.40
3	A	408	ASP	N-CA-C	-7.25	91.44	111.00
3	A	87	GLN	C-N-CA	7.16	139.60	121.70
3	A	407	GLY	N-CA-C	6.51	129.38	113.10
3	A	323	SER	N-CA-CB	6.32	119.98	110.50
4	B	10	GLN	C-N-CA	5.96	136.59	121.70
3	A	401	LYS	CD-CE-NZ	5.86	125.17	111.70
3	A	401	LYS	CB-CG-CD	5.69	126.40	111.60
3	A	492	LYS	CA-C-O	-5.45	108.66	120.10
4	B	10	GLN	O-C-N	-5.27	114.27	122.70
1	G	9	DG	C5'-C4'-C3'	5.26	123.56	114.10
1	G	5	DT	C5'-C4'-C3'	-5.25	104.66	114.10
3	A	324	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	G	10	DG	C5'-C4'-C3'	5.01	123.11	114.10

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
3	A	3636	0	3633	91	0
4	B	1723	0	1710	74	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	182	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 15.

All (182) 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:C	3:A:492:LYS:CA	1.79	1.49
4:B:10:GLN:CA	4:B:10:GLN:C	1.98	1.31
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
1:G:4:DG:H2"	1:G:5:DT:H5"	1.52	0.90
4:B:10:GLN:CB	4:B:10:GLN:C	2.42	0.87
4:B:40:LYS:HD3	4:B:128:ARG:NH2	1.93	0.84
4:B:10:GLN:HA	4:B:10:GLN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:126:GLN:HG3	4:B:128:ARG:HG2	1.80	0.63
4:B:17:LEU:HD11	4:B:35:LEU:HB3	1.79	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
4:B:28:PHE:O	4:B:31:VAL:HG12	1.99	0.62
1:G:5:DT:C2'	1:G:6:DT:H5"	2.13	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
4:B:20:GLU:HB3	4:B:31:VAL:HG23	1.81	0.61
1:H:11:DG:N3	1:H:11:DG:H5'	2.15	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
4:B:47:TYR:CD1	4:B:48:PRO:HA	2.40	0.57
1:G:11:DG:H1'	1:G:12:DG:H5'	1.86	0.57
3:A:124:ARG:NH1	3:A:124:ARG:HG3	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:124:ARG:HG3	3:A:124:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:132:THR:CG2	4:B:133:ARG:N	2.71	0.54
4:B:132:THR:HG22	4:B:133:ARG:N	2.23	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
3:A:230:ILE:HD12	3:A:243:LEU:HG	1.91	0.53
3:A:319:VAL:O	3:A:319:VAL:CG1	2.57	0.52
2:D:10:DG:H2'	2:D:10:DG:N3	2.24	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
4:B:126:GLN:HE21	4:B:128:ARG:CD	2.21	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
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: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
3:A:230:ILE:HD13	3:A:245:LEU:CD2	2.41	0.51
2:D:4:DG:H3'	2:D:4:DG:OP2	2.10	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:323:SER:C	3:A:325:LYS:N	2.63	0.51
1:G:3:DG:N3	1:G:3:DG:H2'	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:230:ILE:HD13	3:A:245:LEU:HD23	1.94	0.50
3:A:48:SER:C	3:A:50:GLN:H	2.15	0.49
3:A:124:ARG:CG	3:A:124:ARG:HH11	2.25	0.49
3:A:492:LYS:C	3:A:492:LYS:HA	2.14	0.49
4:B:92:ASN:HB3	4:B:119:HIS:HB2	1.95	0.49
1:G:9:DG:N3	1:G:9:DG:H2'	2.28	0.49
4:B:220:VAL:HG13	4:B:224:GLY:HA2	1.96	0.48
4:B:81:VAL:HG23	4:B:222:GLU:OE1	2.13	0.48
4:B:212:THR:CG2	4:B:213:LEU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:42:TYR:CE1	4:B:85:ASP:HA	2.48	0.48
3:A:391:ASP:CG	3:A:394:THR:HG22	2.34	0.48
4:B:126:GLN:O	4:B:127:GLU:C	2.52	0.48
3:A:76:LEU:CD2	3:A:76:LEU:N	2.76	0.48
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:323:SER:C	3:A:325:LYS:H	2.16	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: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: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
3:A:429:TYR:CD1	3:A:429:TYR:N	2.83	0.46
3:A:85:LEU:C	3:A:96:ASP:HB2	2.35	0.46
4:B:10:GLN:HB3	4:B:10:GLN:C	2.34	0.46
3:A:338:VAL:CG1	3:A:342:HIS:HB2	2.46	0.46
3:A:399:SER:C	3:A:401:LYS:H	2.20	0.45
3:A:309:LEU:HA	3:A:309:LEU:HD12	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
4:B:127:GLU:O	4:B:129:LEU:HG	2.17	0.45
2:D:8:DT:H2"	2:D:9:DG:H5'	1.98	0.45
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
4:B:81:VAL:O	4:B:81:VAL:HG12	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
3:A:318:SER:C	3:A:320:GLU:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:71:ARG:CZ	3:A:73:ILE:HD11	2.49	0.42
3:A:80:ASP:C	3:A:80:ASP:OD1	2.57	0.42
4:B:209:ASN:N	4:B:209:ASN:OD1	2.47	0.42
4:B:68:VAL:HG11	4:B:218:ILE:HD12	2.01	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:338:VAL:CG1	3:A:339:ASP:N	2.83	0.42
4:B:223:LYS:O	4:B:224:GLY:C	2.57	0.42
4:B:58:PHE:C	4:B:58:PHE:CD1	2.93	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
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
5:D:158:HOH:O	3:A:77:LYS:HE3	2.19	0.41
3:A:400:LEU:HD23	3:A:406:LYS:H	1.85	0.41
3:A:46:LEU:HD22	3:A:129:LEU:HD13	2.02	0.41
3:A:470:LYS:O	3:A:473:SER:HB2	2.21	0.41
3:A:279:ASP:HB2	3:A:289:ILE:HG13	2.02	0.41
4:B:68:VAL:HG23	4:B:69:ASN:N	2.36	0.41
2:D:7:DT:H2'	2:D:7:DT:H6	1.70	0.41
4:B:85:ASP:O	4:B:85:ASP:OD1	2.38	0.41
3:A:124:ARG:NH1	3:A:143:SER:O	2.53	0.41
3:A:71:ARG:NH2	3:A:73:ILE:HD11	2.36	0.41
4:B:126:GLN:H	4:B:126:GLN:HG2	1.71	0.41
4:B:55:GLY:O	4:B:132:THR:HG23	2.20	0.41
3:A:102:LEU:HD23	3:A:138:ALA:HB3	2.02	0.41
3:A:71:ARG:HE	3:A:73:ILE:HD11	1.85	0.41
3:A:232:GLN:NE2	5:A:726:HOH:O	2.27	0.40
4:B:127:GLU:O	4:B:127:GLU:HG3	2.21	0.40
4:B:87:VAL:HG22	4:B:88:ILE:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:63:PHE:O	4:B:212:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	17	29
4	B	213/216 (99%)	189 (89%)	21 (10%)	3 (1%)	13	23
All	All	660/677 (98%)	610 (92%)	42 (6%)	8 (1%)	15	27

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 ⓘ

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%)	385 (96%)	18 (4%)	32	56
4	B	188/189 (100%)	181 (96%)	7 (4%)	39	66
All	All	591/598 (99%)	566 (96%)	25 (4%)	34	59

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	76	LEU
3	A	80	ASP
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	309	LEU
3	A	316	ASP
3	A	324	LEU
3	A	337	GLU
3	A	353	LEU
3	A	398	SER
3	A	416	LEU
3	A	472	ASN
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	92	ASN
4	B	215	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) 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
4	B	10	GLN

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Mol	Chain	Res	Type
4	B	92	ASN
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	0.48	0	8,14,17	0.76	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	-	0/3/15/16	0/1/1/1

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.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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, 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%)	0.05	0	100	100	34, 43, 49, 50	0
1	H	12/13 (92%)	0.18	0	100	100	40, 46, 50, 50	0
2	D	11/12 (91%)	-0.47	0	100	100	25, 34, 52, 52	0
3	A	449/461 (97%)	-0.09	10 (2%)	62	64	17, 29, 49, 60	0
4	B	215/216 (99%)	0.49	20 (9%)	9	9	23, 46, 61, 70	0
All	All	699/715 (97%)	0.09	30 (4%)	36	38	17, 33, 57, 70	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	407	GLY	9.8
4	B	127	GLU	7.6
3	A	406	LYS	6.6
4	B	130	ASN	6.3
4	B	126	GLN	5.9
4	B	129	LEU	5.3
4	B	78	VAL	5.1
3	A	87	GLN	4.8
3	A	70	GLU	4.5
3	A	69	GLN	4.2
4	B	223	LYS	4.2
4	B	196	LYS	3.9
4	B	77	ASN	3.9
4	B	131	PRO	3.9
3	A	319	VAL	3.8
4	B	73	ALA	3.8
4	B	179	ALA	3.6
4	B	224	GLY	3.4
3	A	93	ASP	3.4
4	B	194	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
4	B	206	LYS	2.9
3	A	94	ALA	2.9
3	A	401	LYS	2.7
4	B	132	THR	2.6
4	B	125	LEU	2.4
4	B	128	ARG	2.3
4	B	195	SER	2.3
4	B	60	ALA	2.3
3	A	340	LYS	2.2
4	B	122	LYS	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
2	3DR	D	3	11/12	0.79	0.29	-	50,53,63,68	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.