



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:02 PM UTC

PDB ID : 2HVR / pdb_00002hvr
Title : Structure of T4 RNA Ligase 2 with Nicked 5'-Adenylated nucleic acid duplex containing a 3'-deoxyribonucleotide at the nick
Authors : Nandakumar, J.; Lima, C.D.
Deposited on : 2006-07-30
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
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

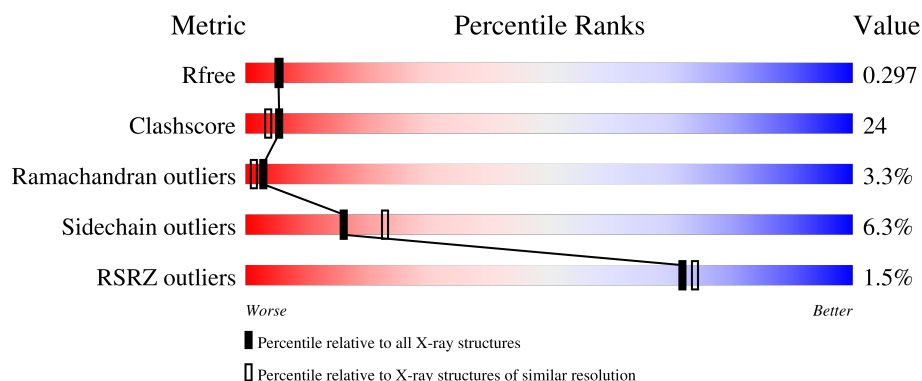
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	C	24	25% 71% .
1	F	24	21% 75% .
2	D	12	17% 58% 25%
2	G	12	25% 58% 17%
3	E	13	31% 62% 8%

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Mol	Chain	Length	Quality of chain
3	H	13	8%92%
4	A	335	%57%32%6%5%
4	B	335	2%54%33%7%5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7219 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(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	24	Total	C	N	O	P	0	0	0
			494	236	91	144	23			
1	F	24	Total	C	N	O	P	0	0	0
			494	236	91	144	23			

- Molecule 2 is DNA/RNA hybrid called 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			241	116	44	70	11			
2	G	12	Total	C	N	O	P	0	0	0
			241	116	44	70	11			

- Molecule 3 is DNA/RNA hybrid called 5'-R(P*A)-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	P	0	0	0
			268	127	50	78	13			
3	H	13	Total	C	N	O	P	0	0	0
			268	127	50	78	13			

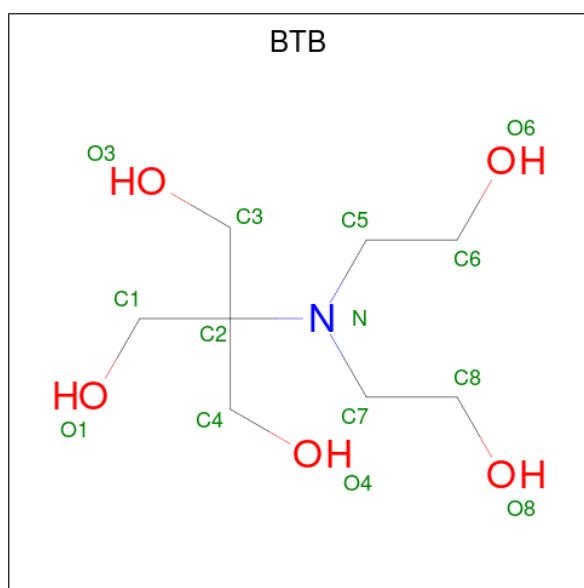
- Molecule 4 is a protein called T4 RNA ligase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	319	Total	C	N	O	S	0	0	0
			2521	1617	409	482	13			
4	B	319	Total	C	N	O	S	0	0	0
			2521	1617	409	482	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP P32277
A	112	GLY	CYS	SEE REMARK 999	UNP P32277
B	0	SER	-	cloning artifact	UNP P32277
B	112	GLY	CYS	SEE REMARK 999	UNP P32277

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	7	Total	O	0	0
			7	7		
6	F	2	Total	O	0	0
			2	2		
6	G	2	Total	O	0	0
			2	2		

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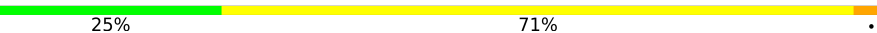
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	2	Total 2	O 2	0	0
6	A	76	Total 76	O 76	0	0
6	B	40	Total 40	O 40	0	0

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.

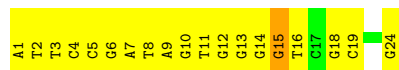
- Molecule 1: 5'-D(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'

Chain C: 

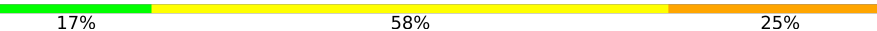


- Molecule 1: 5'-D(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'

Chain F: 



- Molecule 2: 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'

Chain D: 

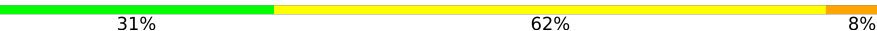


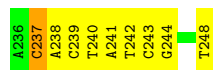
- Molecule 2: 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'

Chain G: 

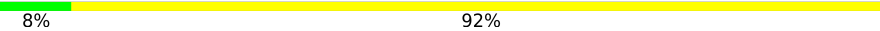


- Molecule 3: 5'-R(P*A)-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'

Chain E: 



- Molecule 3: 5'-R(P*A)-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'

Chain H:  8% 92%

A236
C237
A238
C239
T240
A241
T242
C243
G244
C245
A246
A247
T248

• Molecule 4: T4 RNA ligase 2

Chain A:  57% 32% 6% 5%

S0 M1 Y5 L8 E9 M10 H11 Y12 M13 M14 S14 K15 F16 I17 E18 K19 W30 R33 E34 K35 B47 R55 L60 E69 E70 I71 I85 M86 V91 V92 S93 Y94 Q95 V96 F97 A101 G102 V109 D110 Y111 G112 D113 K114 D115 F116 F119 D120 I121

T124 T125 D129 V130 T131 Y132 Y133 M134 D135 Y136 K137 M138 C142 E146 P151 R155 E159 E160 L161 I162 L164 P165 N166 D167 L168 Q173 D174 Y175 V179 D186 K189 E195 A196 K197 A203 L208 K209 P210 L216 N220 R221 V222 A223

L224 K225 K227 F231 SER GLU LYS LYS SER ASP LYS PRD ILE ALA LYS VAL E246 L247 S248 E249 D250 D251 N252 K253 L254 V255 G256 I257 L258 A259 C260 C261 V262 R266 V270 I271 S272 K273 I274 G275 E276 I277 D280 D281 F282 V285 M286 G287 L288 T289 V290 Q291

L294 E296 T297 S298 R299 E300 G301 T302 T303 L304 T305 D308 R309 I313 K314 K315 E316 L317 V318 K319 M320 D323 V324 L325 R326 P327 A328 W329 T330 E331 L332 VAL SER

• Molecule 4: T4 RNA ligase 2

Chain B:  54% 33% 7% 5%

S0 L8 H11 Y12 M13 S14 K15 F16 I17 E18 K19 L20 Y21 S22 L23 G24 T26 G27 W30 V31 K35 S42 E49 E160 L161 I162 K163 L168 D169 A182 G183 L184 N188 N193 K197 G198 E199 V200 E204 L208 K209 Y212 P213 S214 W215 L216

A101 K107 N108 V109 K114 I122 V123 V124 V130 T131 Y132 V133 D134 Y136 M137 K146 A150 P151 R155 F158 E159 E160 L161 I162 K163 L168 D169 A182 G183 L184 N188 N193 K197 G198 E199 V200 E204 L208 K209 Y212 P213 S214 W215 L216

R217 R218 G219 V222 A223 L224 N228 S229 E230 G301 I302 A307 D308 N309 P310 S311 L312 T313 K314 E315 E316 L317 V318 K319 R320 V321 V324 L325 R326 P327 A328 W329 T330 V333 S334

R217 R218 G219 V222 A223 L224 N228 S229 E230 G301 I302 A307 D308 N309 P310 S311 L312 T313 K314 E315 E316 L317 V318 K319 R320 V321 V324 L325 R326 P327 A328 W329 T330 V333 S334

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.57Å 106.16Å 125.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.45 19.92 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.92-2.45) 98.8 (19.92-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.295 0.238 , 0.297	Depositor DCC
R_{free} test set	2056 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.68% 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: OMC, BTB, O2C

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	C	0.29	0/554	0.69	0/855
1	F	0.30	0/554	0.71	1/855 (0.1%)
2	D	0.27	0/225	0.63	0/345
2	G	0.30	0/225	0.72	0/345
3	E	0.65	1/299 (0.3%)	0.77	0/455
3	H	0.65	1/299 (0.3%)	0.74	0/455
4	A	0.47	0/2570	0.98	10/3472 (0.3%)
4	B	0.46	0/2570	0.99	12/3471 (0.3%)
All	All	0.45	2/7296 (0.0%)	0.91	23/10253 (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
1	C	0	1
1	F	0	2
2	D	0	2
2	G	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	237	DC	OP3-P	5.56	1.59	1.48
3	H	237	DC	OP3-P	5.03	1.58	1.48

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	150	ALA	N-CA-C	-8.48	97.03	109.50
4	A	111	TYR	N-CA-C	-8.41	96.63	110.17
4	A	55	ARG	N-CA-C	6.99	118.90	111.28
4	B	212	TYR	CA-C-N	6.61	128.10	119.84
4	B	212	TYR	C-N-CA	6.61	128.10	119.84
4	A	102	GLY	CA-C-N	6.16	126.52	119.93
4	A	102	GLY	C-N-CA	6.16	126.52	119.93
4	B	209	LYS	N-CA-C	6.11	113.72	108.22
4	A	110	ASP	N-CA-C	6.06	117.32	107.32
4	B	72	LEU	N-CA-C	-5.79	105.10	111.82
4	B	55	ARG	N-CA-C	5.71	117.50	111.28
4	A	146	LYS	N-CA-C	5.69	119.69	111.56
4	B	74	ASN	N-CA-C	5.62	118.34	111.82
1	F	24	DG	C2'-C3'-O3'	-5.60	103.10	111.50
4	A	131	THR	N-CA-C	5.59	117.77	108.99
4	A	135	ASP	N-CA-C	5.57	118.11	111.71
4	B	254	LEU	N-CA-C	-5.36	105.60	111.82
4	B	86	MET	N-CA-C	5.36	116.81	111.07
4	A	60	LEU	CA-C-N	5.25	125.57	119.47
4	A	60	LEU	C-N-CA	5.25	125.57	119.47
4	B	253	LYS	N-CA-C	-5.19	105.80	111.82
4	B	330	ILE	N-CA-C	-5.05	105.57	110.42
4	B	131	THR	N-CA-C	5.04	116.08	108.07

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	14	DG	Sidechain
2	D	133	DA	Sidechain
2	D	134	DC	Sidechain
1	F	14	DG	Sidechain
1	F	15	DG	Sidechain
2	G	133	DA	Sidechain
2	G	134	DC	Sidechain

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	C	494	0	273	26	0
1	F	494	0	273	27	0
2	D	241	0	138	12	0
2	G	241	0	138	10	0
3	E	268	0	148	12	0
3	H	268	0	148	16	0
4	A	2521	0	2511	102	0
4	B	2521	0	2517	119	0
5	A	14	0	19	0	0
5	C	14	0	19	4	0
5	F	14	0	19	4	0
6	A	76	0	0	2	0
6	B	40	0	0	1	0
6	C	7	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	1	0
All	All	7219	0	6203	314	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 24.

All (314) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:DA:H2''	1:C:10:DG:H5''	1.28	1.14
2:G:133:DA:H2''	2:G:134:DC:H5''	1.21	1.13
4:A:251:ASP:HB2	4:A:308:ASP:HB3	1.33	1.10
2:D:133:DA:H2''	2:D:134:DC:H5''	1.16	1.08
4:B:286:MET:HE1	4:B:318:VAL:HG13	1.38	1.06
3:H:241:DA:H2''	3:H:242:DT:H5'	1.42	1.01
1:C:10:DG:H2''	1:C:11:DT:H5'	1.44	0.99
1:C:21:DA:H2''	1:C:22:DT:H5''	1.46	0.97
2:D:133:DA:C2'	2:D:134:DC:H5''	1.96	0.96
4:A:133:VAL:HG12	4:A:137:MET:HB3	1.50	0.94
2:G:133:DA:C2'	2:G:134:DC:H5''	2.00	0.92
4:B:274:ILE:HD11	4:B:288:LEU:HD13	1.52	0.91
4:B:133:VAL:HG13	4:B:137:MET:HB3	1.54	0.89
1:C:9:DA:C2'	1:C:10:DG:H5''	2.04	0.87
4:A:287:GLY:O	4:A:291:GLN:HG2	1.74	0.87
4:B:290:VAL:HG13	4:B:317:LEU:HD12	1.59	0.84
2:D:126:DA:H2''	2:D:127:DA:H5'	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:250:ALA:HA	4:B:253:LYS:HG2	1.59	0.83
4:B:326:ARG:HB2	4:B:327:PRO:HD3	1.61	0.82
3:H:238:DA:H2''	3:H:239:DC:H5''	1.62	0.82
2:D:133:DA:H2''	2:D:134:DC:C5'	2.06	0.81
5:F:202:BTB:H82	2:G:135:OMC:HN42	1.45	0.81
6:H:48:HOH:O	4:B:209:LYS:HE3	1.81	0.80
4:A:315:LYS:O	4:A:318:VAL:HG22	1.81	0.80
4:A:30:TRP:HE3	4:A:208:LEU:HD22	1.47	0.79
2:G:133:DA:H2''	2:G:134:DC:C5'	2.10	0.79
1:F:7:DA:H2''	1:F:8:DT:H5'	1.64	0.78
4:A:274:ILE:HG22	4:A:275:GLY:H	1.48	0.77
4:A:326:ARG:HB3	4:A:327:PRO:HD3	1.67	0.77
4:A:35:LYS:HE3	4:A:227:LYS:HD3	1.67	0.76
4:A:286:MET:HB3	4:A:325:LEU:HD12	1.68	0.76
4:A:16:PHE:HA	4:A:19:LYS:HD3	1.67	0.76
1:C:21:DA:C2'	1:C:22:DT:H5''	2.17	0.75
5:C:201:BTB:C8	2:D:135:OMC:HN42	2.01	0.74
3:H:246:DA:H2''	3:H:247:DA:H5'	1.68	0.74
4:A:162:ILE:HD13	4:A:162:ILE:O	1.88	0.73
3:H:238:DA:H2''	3:H:239:DC:C5'	2.19	0.73
3:H:241:DA:H2''	3:H:242:DT:C5'	2.17	0.73
1:F:15:DG:H2'	1:F:16:DT:C7	2.20	0.72
4:B:159:GLU:H	4:B:159:GLU:CD	1.95	0.72
4:A:133:VAL:CG1	4:A:137:MET:HG2	2.20	0.72
5:C:201:BTB:H82	2:D:135:OMC:HN42	1.55	0.71
1:C:9:DA:H2''	1:C:10:DG:C5'	2.14	0.71
1:F:15:DG:H2'	1:F:16:DT:H72	1.71	0.70
4:A:166:ASN:C	4:A:166:ASN:HD22	1.98	0.70
4:A:331:GLU:O	4:A:332:LEU:HG	1.92	0.70
4:A:166:ASN:HD22	4:A:167:ASP:N	1.89	0.69
4:A:30:TRP:CE3	4:A:208:LEU:HD22	2.27	0.69
4:B:279:PRO:HA	4:B:333:VAL:HG11	1.75	0.69
4:B:290:VAL:HG22	4:B:321:VAL:HG21	1.75	0.69
4:A:253:LYS:HG3	4:A:254:LEU:HD22	1.75	0.68
4:A:266:ARG:O	4:A:270:VAL:HG23	1.93	0.68
3:E:242:DT:H2''	3:E:243:DC:C5	2.29	0.68
4:A:168:LEU:HD13	4:A:203:ALA:HB3	1.75	0.68
1:C:23:DT:H2''	1:C:24:DG:H5'	1.77	0.67
1:C:23:DT:H2''	1:C:24:DG:C5'	2.25	0.67
1:F:9:DA:H2''	1:F:10:DG:H5'	1.77	0.67
4:A:274:ILE:HG22	4:A:275:GLY:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:238:DA:C2'	3:H:239:DC:H5''	2.25	0.66
2:D:130:DG:H1'	2:D:131:DC:H5'	1.77	0.65
1:C:1:DA:H5''	4:B:318:VAL:HG11	1.79	0.65
4:A:257:ILE:O	4:A:260:CYS:HB2	1.98	0.64
1:F:9:DA:H2''	1:F:10:DG:C5'	2.27	0.64
4:B:286:MET:HG3	4:B:287:GLY:N	2.13	0.64
1:F:4:DC:H2''	1:F:5:DC:O5'	1.99	0.63
1:F:18:DG:H4'	1:F:18:DG:OP1	1.99	0.63
4:A:47:ARG:NH1	4:A:91:VAL:O	2.31	0.63
4:A:309:ASN:O	4:A:313:ILE:HG12	1.99	0.63
4:A:304:LEU:HD13	4:A:304:LEU:H	1.63	0.62
4:A:274:ILE:HD11	4:A:288:LEU:HD13	1.81	0.62
1:C:15:DG:H2'	1:C:16:DT:H72	1.81	0.62
4:B:295:GLU:O	4:B:299:ARG:HB2	1.99	0.62
4:B:133:VAL:CG1	4:B:137:MET:HB3	2.28	0.62
4:B:20:LEU:HD23	4:B:25:LEU:HD12	1.81	0.62
4:A:253:LYS:HG3	4:A:254:LEU:N	2.15	0.61
4:B:80:LYS:HE3	4:B:84:ASP:OD2	2.00	0.61
4:B:248:SER:OG	4:B:251:ASP:HB2	1.99	0.60
4:A:133:VAL:HG12	4:A:137:MET:CB	2.27	0.60
4:A:112:GLY:HA3	6:A:362:HOH:O	2.00	0.60
4:A:10:ASN:OD1	4:A:225:LYS:HE3	2.02	0.60
4:B:297:THR:HG23	4:B:298:SER:N	2.15	0.60
1:C:10:DG:C2'	1:C:11:DT:H5'	2.25	0.60
4:A:14:SER:O	4:A:18:GLU:HG2	2.02	0.60
1:F:7:DA:C2'	1:F:8:DT:H5'	2.30	0.59
4:B:193:ASN:N	4:B:193:ASN:HD22	2.00	0.59
3:E:241:DA:H1'	3:E:242:DT:H5'	1.85	0.59
4:A:159:GLU:CD	4:A:159:GLU:H	2.09	0.59
4:B:184:LEU:HG	4:B:188:ASN:ND2	2.18	0.59
4:B:262:VAL:HG12	4:B:324:VAL:HG21	1.85	0.59
4:A:304:LEU:HB2	4:A:314:LYS:HZ3	1.68	0.58
4:A:85:ILE:C	4:A:85:ILE:HD12	2.28	0.58
4:A:262:VAL:HG12	4:A:324:VAL:HG21	1.84	0.58
4:B:279:PRO:CA	4:B:333:VAL:HG11	2.33	0.58
4:A:304:LEU:HD13	4:A:304:LEU:N	2.19	0.58
4:A:166:ASN:C	4:A:166:ASN:ND2	2.61	0.58
4:B:290:VAL:O	4:B:294:LEU:HD22	2.04	0.57
1:C:15:DG:H2'	1:C:16:DT:C7	2.34	0.57
1:F:8:DT:H2''	1:F:9:DA:N7	2.20	0.57
4:B:251:ASP:HA	4:B:308:ASP:OD1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:217:ARG:C	4:B:219:GLY:H	2.14	0.56
2:G:129:DT:H2''	2:G:130:DG:O5'	2.05	0.56
4:B:289:THR:O	4:B:293:ILE:HG13	2.06	0.56
5:F:202:BTB:H82	2:G:135:OMC:N4	2.18	0.56
4:B:229:SER:O	4:B:230:LYS:HB3	2.06	0.56
1:F:7:DA:H1'	1:F:8:DT:C5'	2.36	0.56
4:B:282:PHE:HA	4:B:329:TRP:CZ3	2.40	0.56
4:B:42:SER:HA	4:B:96:VAL:O	2.05	0.56
1:F:6:DG:H2''	1:F:7:DA:H5'	1.88	0.56
4:B:158:PHE:HB3	4:B:159:GLU:OE2	2.06	0.56
4:B:169:ASP:HB3	4:B:200:VAL:HG22	1.88	0.56
4:B:297:THR:CG2	4:B:298:SER:N	2.68	0.55
4:B:94:TYR:CE2	4:B:123:VAL:HG22	2.41	0.55
4:A:308:ASP:O	4:A:309:ASN:HB2	2.05	0.55
4:A:121:ILE:O	4:A:133:VAL:HG23	2.05	0.55
4:A:168:LEU:HD12	4:A:168:LEU:H	1.72	0.55
4:B:30:TRP:HE3	4:B:208:LEU:HD22	1.71	0.55
4:B:259:ALA:CB	4:B:320:MET:HE1	2.37	0.55
3:H:241:DA:H8	3:H:241:DA:OP2	1.90	0.55
4:B:23:LEU:N	4:B:23:LEU:HD12	2.22	0.55
4:B:301:GLY:C	4:B:302:ILE:HD12	2.32	0.55
4:A:314:LYS:H	4:A:314:LYS:HD2	1.72	0.54
1:C:1:DA:O4'	4:B:286:MET:HE2	2.06	0.54
5:C:201:BTB:H81	2:D:135:OMC:HN42	1.70	0.54
4:B:286:MET:CE	4:B:318:VAL:HG13	2.27	0.54
4:A:299:ARG:HG3	4:A:299:ARG:HH11	1.72	0.54
4:A:251:ASP:CB	4:A:308:ASP:HB3	2.22	0.54
4:B:169:ASP:HB3	4:B:200:VAL:CG2	2.38	0.54
4:B:266:ARG:O	4:B:270:VAL:HG23	2.08	0.53
4:B:134:ASP:OD2	4:B:136:TYR:HB2	2.09	0.53
4:B:282:PHE:N	4:B:329:TRP:CH2	2.76	0.53
4:A:71:ILE:HD13	4:A:116:PHE:HB2	1.90	0.53
4:B:17:ILE:O	4:B:20:LEU:HB2	2.09	0.53
4:B:25:LEU:O	4:B:27:GLY:N	2.42	0.53
4:B:229:SER:O	4:B:230:LYS:CB	2.55	0.53
4:A:251:ASP:OD1	4:A:313:ILE:HD11	2.08	0.53
1:F:7:DA:H1'	1:F:8:DT:H5'	1.89	0.53
4:B:302:ILE:HD12	4:B:302:ILE:N	2.24	0.53
4:B:309:ASN:C	4:B:311:SER:H	2.17	0.53
2:G:127:DA:H1'	2:G:128:DT:H5'	1.91	0.52
3:H:239:DC:H2'	3:H:240:DT:H72	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:193:ASN:HD22	4:B:193:ASN:H	1.55	0.52
4:A:251:ASP:C	4:A:253:LYS:H	2.16	0.52
3:E:243:DC:H2''	3:E:244:DG:C8	2.45	0.52
4:B:309:ASN:OD1	4:B:312:LEU:HB3	2.10	0.52
1:F:18:DG:H2'	1:F:19:DC:C6	2.45	0.52
3:H:239:DC:H2''	3:H:240:DT:C6	2.44	0.52
4:A:8:LEU:HB2	4:A:225:LYS:HD3	1.92	0.52
4:A:95:GLN:HG2	4:A:97:PHE:CE1	2.44	0.52
4:A:124:THR:HA	4:A:129:ASP:O	2.09	0.52
4:A:133:VAL:CG1	4:A:137:MET:HB3	2.30	0.52
4:B:314:LYS:O	4:B:318:VAL:HG23	2.10	0.52
4:B:12:TYR:C	4:B:12:TYR:CD1	2.88	0.52
1:F:12:DG:H2''	1:F:13:DG:O5'	2.10	0.51
4:B:132:TYR:O	4:B:213:PRO:HG3	2.11	0.51
1:F:1:DA:N1	3:H:248:DT:O2	2.42	0.51
4:B:259:ALA:HB1	4:B:320:MET:HE1	1.92	0.51
4:B:254:LEU:C	4:B:254:LEU:HD13	2.35	0.51
2:D:125:DC:H2''	2:D:126:DA:O5'	2.11	0.51
4:B:217:ARG:NH1	4:B:217:ARG:HB3	2.25	0.51
1:C:14:DG:H2''	1:C:15:DG:O5'	2.10	0.51
4:B:19:LYS:O	4:B:23:LEU:HD13	2.10	0.51
4:B:155:ARG:O	4:B:155:ARG:HG2	2.11	0.50
4:A:291:GLN:O	4:A:295:GLU:HG3	2.12	0.50
1:C:1:DA:H2''	1:C:2:DT:O5'	2.12	0.50
3:E:237:DC:H2''	3:E:238:DA:H5'	1.94	0.50
1:F:10:DG:H2''	1:F:11:DT:O5'	2.11	0.50
4:B:298:SER:C	4:B:300:GLU:H	2.19	0.50
4:A:248:SER:OG	4:A:251:ASP:HB3	2.11	0.50
4:B:25:LEU:C	4:B:27:GLY:H	2.18	0.50
1:C:1:DA:C8	4:B:318:VAL:HG21	2.47	0.50
3:E:248:DT:H71	4:B:314:LYS:NZ	2.27	0.50
4:B:193:ASN:H	4:B:193:ASN:ND2	2.09	0.50
4:B:294:LEU:HA	4:B:297:THR:HG22	1.94	0.50
4:B:254:LEU:HD13	4:B:254:LEU:O	2.11	0.49
4:B:161:LEU:C	4:B:163:LYS:H	2.19	0.49
2:G:125:DC:H2''	2:G:126:DA:O5'	2.11	0.49
4:B:249:GLU:O	4:B:250:ALA:HB2	2.12	0.49
1:C:6:DG:H2''	1:C:7:DA:C8	2.48	0.49
1:C:9:DA:C3'	1:C:10:DG:H5''	2.39	0.49
4:B:298:SER:C	4:B:300:GLU:N	2.70	0.49
4:B:247:LEU:N	4:B:247:LEU:HD23	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:DT:H2''	1:F:3:DT:O5'	2.13	0.48
4:B:302:ILE:O	4:B:302:ILE:HG22	2.13	0.48
4:A:216:LEU:HD12	4:A:220:ASN:HB2	1.95	0.48
4:A:257:ILE:HG22	4:A:258:LEU:N	2.28	0.48
2:D:130:DG:H2''	2:D:131:DC:O5'	2.14	0.48
4:A:304:LEU:HD22	4:A:305:THR:N	2.29	0.48
5:F:202:BTB:C8	2:G:135:OMC:HN42	2.22	0.48
4:B:123:VAL:HG23	4:B:133:VAL:HG23	1.96	0.48
1:F:1:DA:H61	3:H:248:DT:H3	1.61	0.48
2:G:134:DC:H2''	2:G:135:OMC:H6	1.79	0.47
4:A:275:GLY:O	4:A:277:ILE:HG13	2.14	0.47
4:B:168:LEU:HD12	4:B:168:LEU:N	2.30	0.47
4:A:133:VAL:HG13	4:A:137:MET:HG2	1.95	0.47
4:A:137:MET:HE3	6:A:370:HOH:O	2.14	0.47
4:A:168:LEU:HD12	4:A:168:LEU:N	2.29	0.47
4:A:186:ASP:OD1	4:A:189:LYS:NZ	2.48	0.47
4:B:252:ASN:O	4:B:255:VAL:HB	2.15	0.47
1:C:18:DG:H2''	1:C:19:DC:O5'	2.15	0.47
4:A:294:LEU:O	4:A:297:THR:HG22	2.14	0.47
4:B:72:LEU:O	4:B:76:ALA:HB2	2.14	0.47
4:B:313:ILE:HG22	4:B:314:LYS:N	2.30	0.47
1:F:6:DG:H2''	1:F:7:DA:C5'	2.45	0.47
3:H:244:DG:H2''	3:H:245:DG:C8	2.50	0.47
4:A:175:TYR:O	4:A:179:VAL:HG23	2.14	0.47
1:C:21:DA:H2''	1:C:22:DT:C5'	2.31	0.47
4:A:254:LEU:O	4:A:257:ILE:N	2.48	0.47
1:F:7:DA:H2''	1:F:8:DT:OP2	2.15	0.46
4:A:251:ASP:C	4:A:253:LYS:N	2.73	0.46
4:A:286:MET:HG3	4:A:287:GLY:N	2.30	0.46
4:B:161:LEU:C	4:B:163:LYS:N	2.73	0.46
3:E:242:DT:H2''	3:E:243:DC:C6	2.50	0.46
1:F:10:DG:H1	3:H:239:DC:H42	1.62	0.46
4:A:282:PHE:CE1	4:A:325:LEU:HD13	2.51	0.46
4:B:69:GLU:H	4:B:69:GLU:CD	2.21	0.46
1:C:19:DC:H2''	1:C:20:DA:OP2	2.16	0.46
4:A:12:TYR:O	4:A:14:SER:N	2.49	0.46
4:A:33:ARG:HH11	4:A:135:ASP:CG	2.24	0.46
4:B:18:GLU:HA	4:B:21:TYR:HD1	1.79	0.46
4:B:20:LEU:CD2	4:B:25:LEU:HD12	2.45	0.46
4:B:274:ILE:O	4:B:275:GLY:C	2.59	0.46
4:A:308:ASP:O	4:A:308:ASP:CG	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:259:ALA:HB2	4:A:320:MET:HE1	1.98	0.46
4:B:146:LYS:HA	4:B:184:LEU:CD2	2.46	0.46
4:B:217:ARG:C	4:B:219:GLY:N	2.74	0.46
4:B:274:ILE:O	4:B:276:GLU:N	2.49	0.46
3:H:236:A:H5''	4:B:8:LEU:HD12	1.98	0.45
4:A:163:LYS:O	4:A:164:LEU:C	2.59	0.45
4:B:193:ASN:N	4:B:193:ASN:ND2	2.64	0.45
4:A:320:MET:O	4:A:324:VAL:HG23	2.16	0.45
4:B:216:LEU:O	4:B:218:ASN:N	2.50	0.45
4:B:130:VAL:O	4:B:131:THR:HB	2.17	0.45
4:B:286:MET:HG3	4:B:287:GLY:H	1.79	0.45
4:B:278:GLY:C	4:B:280:LYS:H	2.24	0.45
4:A:248:SER:O	4:A:252:ASN:HB2	2.17	0.45
4:A:254:LEU:O	4:A:255:VAL:C	2.60	0.45
4:B:25:LEU:C	4:B:27:GLY:N	2.72	0.45
4:A:259:ALA:CB	4:A:320:MET:HE1	2.47	0.45
4:A:281:ASP:O	4:A:285:VAL:HG23	2.15	0.45
2:D:134:DC:H2''	2:D:135:OMC:H6	1.82	0.45
4:A:1:MET:HE2	4:A:93:SER:OG	2.16	0.45
4:B:71:ILE:HD11	4:B:100:PHE:CD1	2.52	0.45
4:B:298:SER:HA	4:B:302:ILE:C	2.41	0.45
4:B:107:LYS:O	4:B:109:VAL:HG22	2.16	0.45
4:B:271:ILE:HG23	4:B:277:ILE:CD1	2.46	0.45
4:B:307:ALA:O	4:B:308:ASP:C	2.60	0.45
2:D:128:DT:H2''	2:D:129:DT:O5'	2.16	0.44
4:B:31:VAL:O	4:B:208:LEU:HD23	2.17	0.44
1:F:9:DA:H1'	1:F:10:DG:H5''	1.98	0.44
4:A:133:VAL:CG1	4:A:137:MET:CG	2.94	0.44
4:A:330:ILE:C	4:A:332:LEU:H	2.26	0.44
3:E:237:DC:C2'	3:E:238:DA:H5'	2.47	0.44
4:A:285:VAL:HG21	4:A:329:TRP:CZ3	2.53	0.44
4:B:14:SER:O	4:B:15:LYS:C	2.60	0.44
1:F:7:DA:C1'	1:F:8:DT:H5'	2.47	0.44
3:E:239:DC:C2'	3:E:240:DT:H71	2.48	0.44
4:A:119:PHE:HA	4:A:138:MET:HE1	1.99	0.44
4:A:257:ILE:O	4:A:260:CYS:CB	2.64	0.44
4:A:247:LEU:HD22	4:A:252:ASN:OD1	2.18	0.43
4:A:319:LYS:HG2	4:A:323:ASP:OD2	2.17	0.43
4:B:216:LEU:O	4:B:217:ARG:C	2.61	0.43
4:A:86:MET:HE1	4:A:93:SER:HA	1.99	0.43
4:A:111:TYR:O	4:A:112:GLY:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:30:TRP:O	4:A:155:ARG:HA	2.18	0.43
4:B:12:TYR:C	4:B:12:TYR:HD1	2.24	0.43
4:B:274:ILE:O	4:B:274:ILE:HG22	2.18	0.43
4:A:125:THR:OG1	4:A:129:ASP:HB2	2.19	0.43
4:A:308:ASP:O	4:A:309:ASN:CB	2.66	0.43
4:B:85:ILE:HD12	4:B:85:ILE:C	2.43	0.43
4:B:214:SER:OG	4:B:222:VAL:HG21	2.17	0.43
1:F:7:DA:H1'	1:F:8:DT:H5''	2.01	0.43
4:A:326:ARG:C	4:A:328:ALA:H	2.26	0.43
4:B:228:ASN:HD22	4:B:230:LYS:N	2.17	0.43
4:B:122:ILE:HD11	4:B:132:TYR:CZ	2.55	0.42
4:A:101:ALA:O	4:A:114:LYS:HA	2.19	0.42
1:C:22:DT:H2'	1:C:23:DT:H72	1.99	0.42
1:F:8:DT:H2''	1:F:9:DA:C8	2.54	0.42
4:B:101:ALA:O	4:B:114:LYS:HA	2.19	0.42
4:B:35:LYS:HG2	4:B:204:GLU:OE1	2.20	0.42
1:C:5:DC:H42	3:E:244:DG:H1	1.68	0.42
4:A:5:TYR:HB2	4:A:97:PHE:CE2	2.54	0.42
4:B:11:HIS:HA	4:B:224:ILE:HG21	2.01	0.42
4:B:86:MET:N	6:B:344:HOH:O	2.52	0.42
4:A:142:CYS:O	4:A:146:LYS:N	2.53	0.42
4:A:301:GLY:O	4:A:303:THR:N	2.53	0.42
3:E:241:DA:H2''	3:E:242:DT:O5'	2.20	0.41
3:H:239:DC:H2''	3:H:240:DT:H6	1.84	0.41
4:B:60:LEU:HA	4:B:61:PRO:HD3	1.95	0.41
4:B:298:SER:HA	4:B:302:ILE:O	2.20	0.41
1:C:14:DG:O6	5:C:201:BTB:H62	2.21	0.41
1:C:23:DT:H2''	1:C:24:DG:H5''	1.99	0.41
4:B:286:MET:HB3	4:B:325:LEU:HD12	2.03	0.41
4:A:224:ILE:HG22	4:A:225:LYS:N	2.35	0.41
4:A:272:SER:C	4:A:274:ILE:H	2.29	0.41
4:B:20:LEU:HB3	4:B:26:THR:HG23	2.03	0.41
4:A:195:GLU:OE1	4:A:197:LYS:HE3	2.21	0.41
3:H:240:DT:H2''	3:H:241:DA:OP2	2.21	0.41
3:E:243:DC:H2''	3:E:244:DG:OP2	2.20	0.41
1:F:1:DA:H2''	1:F:2:DT:OP2	2.20	0.41
4:A:286:MET:HE3	4:A:286:MET:O	2.21	0.41
4:B:217:ARG:HB3	4:B:217:ARG:CZ	2.51	0.41
4:B:316:GLU:HA	4:B:316:GLU:OE1	2.20	0.41
3:E:239:DC:H2''	3:E:240:DT:H71	2.02	0.41
4:A:35:LYS:CE	4:A:227:LYS:HD3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:297:THR:CG2	4:B:298:SER:H	2.34	0.41
4:B:326:ARG:HB2	4:B:327:PRO:CD	2.41	0.41
1:C:2:DT:H5'	4:B:287:GLY:HA3	2.03	0.41
4:A:161:LEU:C	4:A:163:LYS:N	2.78	0.41
4:A:290:VAL:O	4:A:294:LEU:HD23	2.21	0.40
4:A:210:PRO:HD3	4:A:222:VAL:O	2.21	0.40
4:B:212:TYR:HA	4:B:213:PRO:HD2	1.75	0.40
4:A:220:ASN:HD22	4:A:220:ASN:HA	1.65	0.40
1:F:13:DG:N7	5:F:202:BTB:H51	2.36	0.40
4:B:91:VAL:HG13	4:B:123:VAL:HG13	2.04	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	
4	A	315/335 (94%)	277 (88%)	29 (9%)	9 (3%)	3	2
4	B	315/335 (94%)	272 (86%)	31 (10%)	12 (4%)	2	1
All	All	630/670 (94%)	549 (87%)	60 (10%)	21 (3%)	3	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	309	ASN
4	B	250	ALA
4	B	275	GLY
4	A	13	ASN
4	A	112	GLY
4	A	302	ILE
4	B	26	THR
4	B	213	PRO

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Mol	Chain	Res	Type
4	B	217	ARG
4	A	250	ALA
4	B	197	LYS
4	B	198	GLY
4	B	218	ASN
4	B	308	ASP
4	B	310	PRO
4	A	285	VAL
4	B	274	ILE
4	A	151	PRO
4	A	313	ILE
4	A	327	PRO
4	B	279	PRO

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	
4	A	277/293 (94%)	257 (93%)	20 (7%)	13	17
4	B	278/293 (95%)	263 (95%)	15 (5%)	20	29
All	All	555/586 (95%)	520 (94%)	35 (6%)	16	23

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	47	ARG
4	A	69	GLU
4	A	109	VAL
4	A	115	ASP
4	A	129	ASP
4	A	131	THR
4	A	162	ILE
4	A	166	ASN
4	A	168	LEU
4	A	173	GLN

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Mol	Chain	Res	Type
4	A	208	LEU
4	A	253	LYS
4	A	257	ILE
4	A	280	LYS
4	A	286	MET
4	A	300	GLU
4	A	304	LEU
4	A	309	ASN
4	A	317	LEU
4	A	325	LEU
4	B	47	ARG
4	B	49	LYS
4	B	69	GLU
4	B	72	LEU
4	B	151	PRO
4	B	155	ARG
4	B	159	GLU
4	B	162	ILE
4	B	168	LEU
4	B	169	ASP
4	B	193	ASN
4	B	208	LEU
4	B	218	ASN
4	B	288	LEU
4	B	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	166	ASN
4	A	173	GLN
4	A	193	ASN
4	A	220	ASN
4	A	268	ASN
4	A	322	GLN
4	B	83	GLN
4	B	173	GLN
4	B	181	HIS
4	B	193	ASN
4	B	220	ASN
4	B	228	ASN
4	B	268	ASN

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Mol	Chain	Res	Type
4	B	322	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are 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	O2C	D	136	2	16,20,21	0.44	0	20,28,31	0.41	0
2	OMC	G	135	2,1	19,22,23	0.69	0	25,31,34	0.75	0
2	O2C	G	136	2	16,20,21	0.41	0	20,28,31	0.47	0
2	OMC	D	135	2,1	19,22,23	0.68	0	25,31,34	0.97	2 (8%)

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	O2C	D	136	2	-	0/7/21/22	0/2/2/2
2	OMC	G	135	2,1	-	0/9/27/28	0/2/2/2
2	O2C	G	136	2	-	0/7/21/22	0/2/2/2
2	OMC	D	135	2,1	-	1/9/27/28	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	135	OMC	CM2-O2'-C2'	-3.13	106.43	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	135	OMC	C5'-C4'-C3'	-2.05	107.84	115.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	135	OMC	C3'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	135	OMC	4	0
2	D	135	OMC	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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	$\# Z > 2$
5	BTB	A	335	-	13,13,13	2.41	2 (15%)	7,16,16	1.94	3 (42%)
5	BTB	F	202	-	13,13,13	2.31	3 (23%)	7,16,16	1.78	3 (42%)
5	BTB	C	201	-	13,13,13	2.37	3 (23%)	7,16,16	1.84	2 (28%)

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
5	BTB	A	335	-	-	8/21/21/21	-
5	BTB	F	202	-	-	4/21/21/21	-
5	BTB	C	201	-	-	5/21/21/21	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	BTB	C5-N	5.85	1.56	1.48
5	A	335	BTB	C5-N	5.84	1.56	1.48
5	F	202	BTB	C5-N	5.80	1.56	1.48
5	A	335	BTB	C2-N	5.55	1.59	1.48
5	C	201	BTB	C2-N	5.25	1.58	1.48
5	F	202	BTB	C2-N	4.99	1.58	1.48
5	C	201	BTB	C7-N	2.46	1.51	1.48
5	F	202	BTB	C7-N	2.20	1.51	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	201	BTB	C8-C7-N	2.87	122.81	111.59
5	F	202	BTB	C8-C7-N	2.84	122.69	111.59
5	A	335	BTB	O3-C3-C2	-2.80	104.83	111.40
5	A	335	BTB	C8-C7-N	2.75	122.31	111.59
5	C	201	BTB	O3-C3-C2	-2.49	105.56	111.40
5	A	335	BTB	C6-C5-N	2.26	120.41	111.59
5	F	202	BTB	O3-C3-C2	-2.17	106.29	111.40
5	F	202	BTB	C6-C5-N	2.12	119.88	111.59

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	201	BTB	C1-C2-N-C7
5	C	201	BTB	C3-C2-N-C7
5	C	201	BTB	C4-C2-N-C7
5	F	202	BTB	C1-C2-N-C7
5	F	202	BTB	C3-C2-N-C7
5	F	202	BTB	C4-C2-N-C7
5	A	335	BTB	C1-C2-N-C7
5	A	335	BTB	C3-C2-N-C7

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Mol	Chain	Res	Type	Atoms
5	A	335	BTB	C4-C2-N-C7
5	F	202	BTB	N-C5-C6-O6
5	A	335	BTB	N-C7-C8-O8
5	C	201	BTB	N-C7-C8-O8
5	C	201	BTB	N-C5-C6-O6
5	A	335	BTB	O1-C1-C2-C4
5	A	335	BTB	N-C5-C6-O6
5	A	335	BTB	O1-C1-C2-C3
5	A	335	BTB	O1-C1-C2-N

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	202	BTB	4	0
5	C	201	BTB	4	0

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	C	24/24 (100%)	0.56	0	100	100	52, 91, 124, 130	0
1	F	24/24 (100%)	0.44	0	100	100	48, 74, 150, 161	0
2	D	10/12 (83%)	0.45	0	100	100	60, 101, 121, 123	0
2	G	10/12 (83%)	0.42	0	100	100	63, 74, 90, 93	0
3	E	13/13 (100%)	0.32	0	100	100	38, 91, 118, 126	0
3	H	13/13 (100%)	0.50	0	100	100	38, 94, 141, 146	0
4	A	319/335 (95%)	-0.20	4 (1%)	75	77	18, 47, 103, 122	0
4	B	319/335 (95%)	-0.04	7 (2%)	62	64	23, 52, 110, 127	0
All	All	732/768 (95%)	-0.04	11 (1%)	72	74	18, 54, 114, 161	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	219	GLY	6.0
4	A	277	ILE	3.7
4	B	247	LEU	3.0
4	B	182	ALA	3.0
4	A	231	PHE	2.9
4	A	196	ALA	2.6
4	B	277	ILE	2.5
4	A	332	LEU	2.5
4	B	333	VAL	2.1
4	B	21	TYR	2.0
4	B	308	ASP	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	OMC	D	135	21/22	0.95	0.08	32,41,46,49	0
2	OMC	G	135	21/22	0.95	0.07	24,40,48,55	0
2	O2C	D	136	19/20	0.97	0.07	23,36,46,48	0
2	O2C	G	136	19/20	0.97	0.06	34,38,46,47	0

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(Å ²)	Q<0.9
5	BTB	A	335	14/14	0.73	0.15	110,114,117,119	0
5	BTB	C	201	14/14	0.78	0.22	74,81,92,96	0
5	BTB	F	202	14/14	0.80	0.28	60,81,84,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.