



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:11 PM GMT

PDB ID : 4O26
Title : Crystal structure of the TRBD domain of TERT and the CR4/5 of TR
Authors : Huang, J.; Wu, J.; Lei, M.
Deposited on : 2013-12-16
Resolution : 3.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

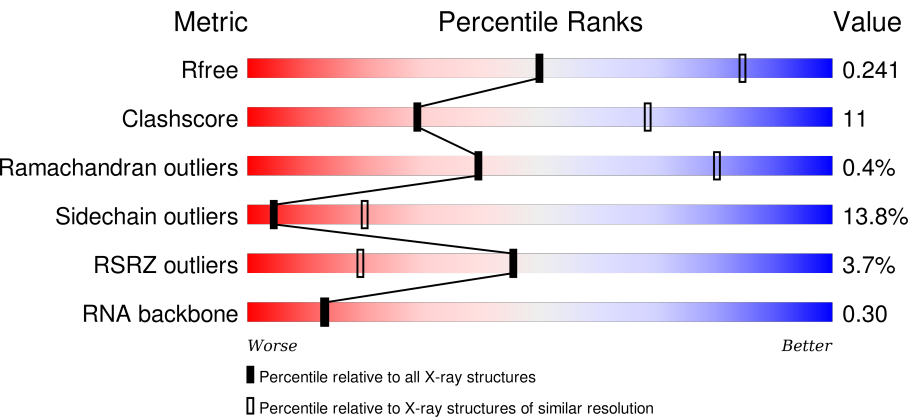
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	A	257	<div><div></div><div>63%28%7%</div></div>
1	B	257	<div><div>3%</div><div>59%24%6%11%</div></div>
2	E	51	<div><div>4%</div><div>33%29%27%8%</div></div>
2	F	51	<div><div>20%</div><div>33%35%22%8%</div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	601	-	-	X	-
3	SO4	A	603	-	-	-	X
3	SO4	A	608	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5940 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 protein called Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1965	1261	371	320	13			
1	B	228	Total	C	N	O	S	0	0	0
			1884	1214	354	304	12			

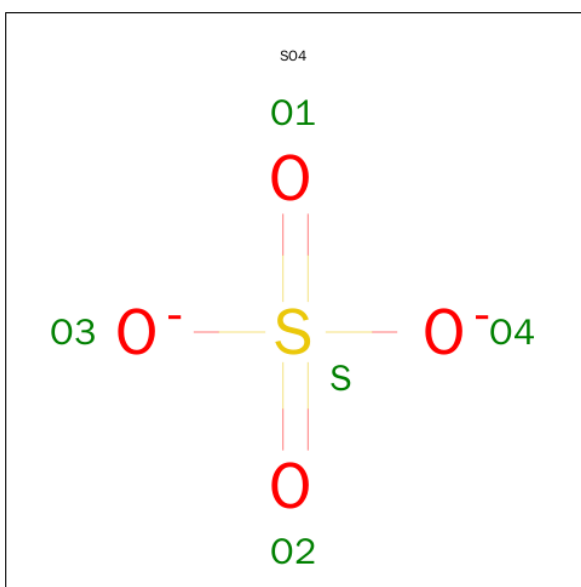
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	GLY	-	EXPRESSION TAG	UNP Q1PS67
A	317	SER	-	EXPRESSION TAG	UNP Q1PS67
B	316	GLY	-	EXPRESSION TAG	UNP Q1PS67
B	317	SER	-	EXPRESSION TAG	UNP Q1PS67

- Molecule 2 is a RNA chain called Telomerase TR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	47	Total	C	N	O	P	0	0	0
			1000	445	174	334	47			
2	F	47	Total	C	N	O	P	0	0	0
			1000	445	174	334	47			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

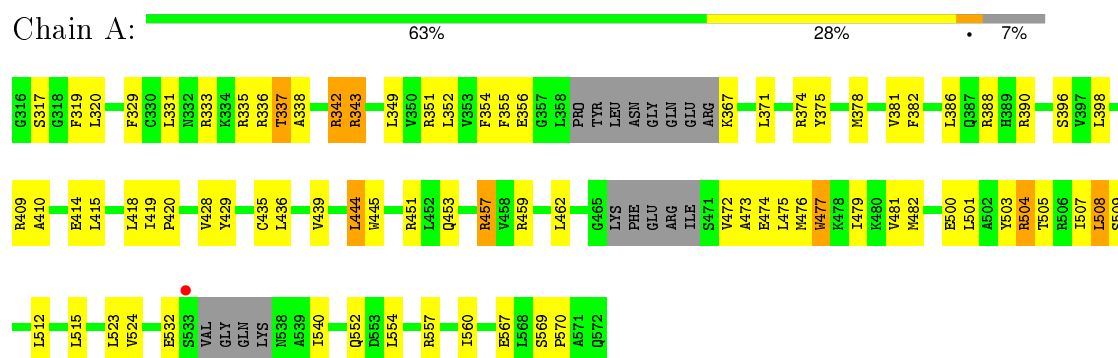
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	8	Total 8	O 8	0	0
4	E	2	Total 2	O 2	0	0

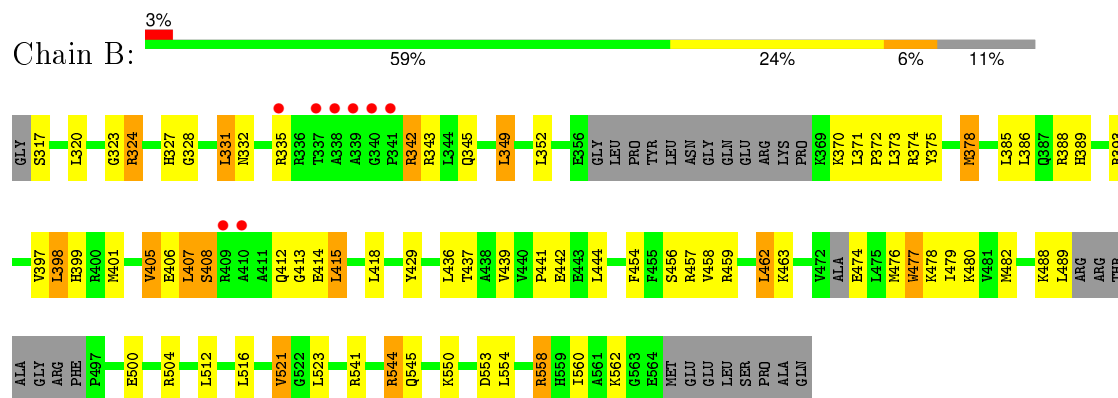
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

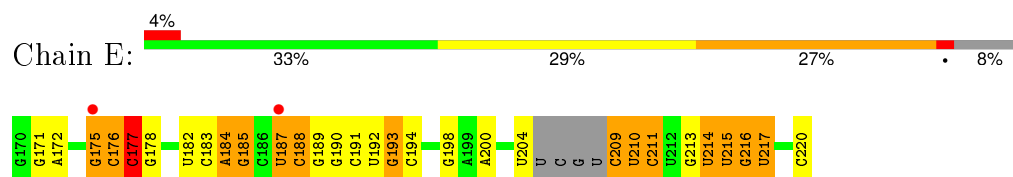
• Molecule 1: Telomerase reverse transcriptase



• Molecule 1: Telomerase reverse transcriptase

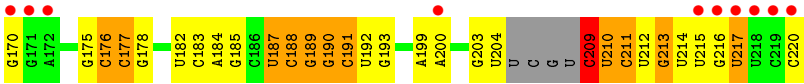


• Molecule 2: Telomerase TR



• Molecule 2: Telomerase TR





4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.09Å 118.09Å 358.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.97 – 3.00 41.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.97-3.00) 99.9 (41.97-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.221 , 0.261 0.227 , 0.241	Depositor DCC
R_{free} test set	1543 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 30534 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5940	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

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	A	0.40	0/2012	0.60	0/2702
1	B	0.33	0/1929	0.56	0/2588
2	E	0.35	0/1114	0.89	1/1732 (0.1%)
2	F	0.24	0/1114	0.87	2/1732 (0.1%)
All	All	0.34	0/6169	0.71	3/8754 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	187	U	C2-N1-C1'	6.32	125.28	117.70
2	E	177	C	O4'-C1'-N1	5.33	112.47	108.20
2	F	209	C	P-O3'-C3'	5.30	126.06	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	477	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	B	477	TRP	Peptide

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	A	1965	0	1996	47	0
1	B	1884	0	1920	45	0
2	E	1000	0	508	20	1
2	F	1000	0	508	13	1
3	A	40	0	0	4	0
3	B	20	0	0	1	0
4	A	21	0	0	0	0
4	B	8	0	0	0	0
4	E	2	0	0	0	0
All	All	5940	0	4932	119	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (119) 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:A:481:VAL:HG21	1:A:505:THR:HG22	1.53	0.89
2:F:209:C:HO2'	2:F:210:U:H6	1.28	0.80
1:B:332:ASN:OD1	1:B:389:HIS:NE2	2.16	0.77
1:B:323:GLY:O	1:B:545:GLN:NE2	2.19	0.75
1:A:532:GLU:HG2	1:A:540:ILE:HG13	1.70	0.74
1:B:415:LEU:HD12	1:B:554:LEU:HD13	1.70	0.73
1:A:342:ARG:HD3	1:A:343:ARG:H	1.58	0.69
1:B:477:TRP:HE3	1:B:479:ILE:HB	1.60	0.65
1:B:374:ARG:NH2	1:B:500:GLU:OE1	2.27	0.63
2:F:170:G:H1	2:F:220:C:H42	1.48	0.61
1:B:477:TRP:CE3	1:B:479:ILE:HB	2.35	0.60
1:B:371:LEU:O	2:F:189:G:N1	2.35	0.60
2:F:209:C:O2'	2:F:210:U:O5'	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:NH2	3:A:601:SO4:O4	2.34	0.60
1:A:390:ARG:NH2	3:A:601:SO4:O2	2.34	0.60
2:E:209:C:O2'	2:E:210:U:OP1	2.18	0.60
2:E:191:C:N4	2:E:192:U:O4	2.36	0.59
1:B:408:SER:HB3	1:B:412:GLN:HA	1.86	0.58
1:A:351:ARG:HD3	1:A:367:LYS:HB3	1.86	0.58
1:B:405:VAL:HG12	1:B:406:GLU:H	1.68	0.58
2:F:176:C:N4	2:F:217:U:O2	2.37	0.57
1:A:342:ARG:HD3	1:A:343:ARG:N	2.19	0.56
1:B:558:ARG:HH11	1:B:558:ARG:HB3	1.70	0.56
1:B:480:LYS:NZ	2:F:212:U:OP1	2.38	0.56
1:A:374:ARG:NH2	1:A:500:GLU:OE1	2.38	0.56
1:A:451:ARG:NH2	1:B:553:ASP:OD2	2.40	0.55
1:B:349:LEU:HD11	1:B:385:LEU:HD22	1.87	0.55
1:B:558:ARG:HH12	1:B:560:ILE:HD13	1.72	0.54
1:A:388:ARG:HB3	1:A:439:VAL:HA	1.89	0.54
1:A:319:PHE:HB2	1:A:524:VAL:HG22	1.89	0.54
1:B:408:SER:HA	1:B:413:GLY:H	1.73	0.53
1:A:554:LEU:HD23	1:A:557:ARG:NH1	2.23	0.53
1:B:331:LEU:HB3	1:B:389:HIS:CD2	2.43	0.53
2:F:177:C:N3	2:F:217:U:H1'	2.23	0.53
1:B:398:LEU:HD13	1:B:544:ARG:CZ	2.39	0.53
1:B:349:LEU:HD12	1:B:386:LEU:HG	1.91	0.53
2:F:210:U:H2'	2:F:211:C:C6	2.44	0.52
1:B:441:PRO:HD2	1:B:444:LEU:HD23	1.92	0.52
1:A:473:ALA:O	1:A:477:TRP:NE1	2.37	0.52
2:F:188:C:O2'	2:F:190:G:N1	2.39	0.52
1:B:442:GLU:N	1:B:442:GLU:OE1	2.40	0.52
1:A:501:LEU:O	1:A:505:THR:HG23	2.09	0.51
1:A:390:ARG:NE	3:A:601:SO4:O2	2.43	0.51
1:A:335:ARG:CZ	1:A:342:ARG:HB3	2.42	0.50
1:A:351:ARG:HG3	1:A:371:LEU:HD21	1.94	0.50
2:E:187:U:H4'	2:E:188:C:OP2	2.12	0.50
1:B:418:LEU:HD21	1:B:550:LYS:HB3	1.93	0.50
2:F:211:C:H2'	2:F:212:U:C6	2.47	0.50
2:E:177:C:N3	2:E:217:U:H1'	2.26	0.50
1:A:477:TRP:HZ3	1:A:508:LEU:HD13	1.76	0.49
2:E:210:U:H2'	2:E:211:C:C6	2.48	0.49
1:B:399:HIS:ND1	3:B:603:SO4:O2	2.44	0.49
1:B:405:VAL:O	1:B:407:LEU:HG	2.13	0.49
1:A:472:VAL:HG22	1:A:475:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:210:U:O2'	2:E:211:C:OP1	2.28	0.49
2:E:176:C:C2'	2:E:177:C:H5'	2.43	0.48
1:A:482:MET:HE1	1:A:504:ARG:HH21	1.78	0.48
2:E:213:G:N2	2:E:214:U:O2	2.46	0.48
2:E:188:C:OP2	2:E:188:C:H4'	2.12	0.48
2:E:175:G:HO2'	2:E:176:C:H6	1.59	0.48
1:A:445:TRP:CE2	1:A:451:ARG:HG3	2.48	0.48
1:B:463:LYS:HE3	1:B:463:LYS:HB2	1.72	0.48
1:B:388:ARG:HB3	1:B:439:VAL:HA	1.96	0.47
1:A:335:ARG:HG2	1:A:342:ARG:O	2.14	0.47
1:A:476:MET:C	1:A:477:TRP:CD1	2.88	0.47
1:A:349:LEU:HD23	1:A:382:PHE:HB3	1.97	0.47
1:A:457:ARG:NH2	1:A:475:LEU:O	2.48	0.47
1:B:373:LEU:HD23	1:B:489:LEU:HD11	1.97	0.47
1:B:374:ARG:HH21	1:B:504:ARG:HD3	1.79	0.47
1:A:435:CYS:O	1:A:439:VAL:HG13	2.15	0.46
1:B:370:LYS:O	1:B:372:PRO:HD3	2.15	0.46
1:A:351:ARG:HA	1:A:355:PHE:HD2	1.81	0.46
2:F:210:U:HO2'	2:F:211:C:P	2.39	0.46
1:B:516:LEU:O	1:B:521:VAL:HG13	2.15	0.45
2:E:217:U:H3'	2:E:217:U:OP1	2.17	0.45
2:E:184:A:H2'	2:E:185:G:C8	2.51	0.45
2:E:175:G:O2'	2:E:176:C:H6	1.99	0.45
1:B:474:GLU:C	1:B:476:MET:H	2.20	0.45
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.83	0.45
1:B:482:MET:HB2	2:F:213:G:OP1	2.17	0.45
1:A:329:PHE:CE2	1:A:331:LEU:HB2	2.52	0.45
1:B:454:PHE:O	1:B:458:VAL:HG23	2.15	0.45
1:A:429:TYR:OH	3:A:607:SO4:O4	2.27	0.45
1:B:429:TYR:CE1	1:B:459:ARG:HB2	2.52	0.45
1:A:569:SER:HA	1:A:570:PRO:HD3	1.73	0.45
1:A:451:ARG:HH22	1:B:553:ASP:CG	2.19	0.45
1:A:459:ARG:HD3	1:B:324:ARG:NH1	2.32	0.45
2:E:184:A:H2'	2:E:185:G:H8	1.82	0.45
1:A:375:TYR:O	1:A:378:MET:HG2	2.17	0.45
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.84	0.45
1:B:523:LEU:HD23	1:B:523:LEU:HA	1.84	0.45
1:A:342:ARG:HH11	1:A:342:ARG:HA	1.82	0.44
1:A:554:LEU:HD23	1:A:557:ARG:HH12	1.81	0.44
1:B:393:ARG:O	1:B:397:VAL:HG23	2.18	0.44
2:E:193:G:H2'	2:E:194:C:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HD3	1:B:343:ARG:H	1.82	0.44
1:A:477:TRP:CE3	1:A:479:ILE:HB	2.52	0.44
1:B:436:LEU:HA	1:B:436:LEU:HD12	1.84	0.44
1:A:354:PHE:CE1	1:A:507:ILE:HG23	2.53	0.44
1:B:512:LEU:HA	1:B:512:LEU:HD12	1.81	0.44
2:F:191:C:N4	2:F:192:U:O4	2.51	0.43
1:A:419:ILE:HA	1:A:420:PRO:HD3	1.85	0.42
1:A:477:TRP:HZ2	1:A:509:SER:HB3	1.83	0.42
1:A:335:ARG:NH1	1:A:343:ARG:O	2.52	0.42
1:B:462:LEU:HA	1:B:462:LEU:HD12	1.85	0.42
1:A:472:VAL:CG2	1:A:475:LEU:HB2	2.49	0.42
2:E:213:G:C2	2:E:214:U:O2	2.72	0.42
1:A:336:ARG:O	1:A:338:ALA:N	2.53	0.42
1:A:375:TYR:OH	1:A:503:TYR:OH	2.38	0.41
2:E:215:U:O2'	2:E:216:G:H5'	2.20	0.41
1:B:335:ARG:HH22	1:B:345:GLN:NE2	2.19	0.41
1:B:374:ARG:NH2	1:B:504:ARG:HH11	2.17	0.41
2:E:176:C:H2'	2:E:177:C:H5'	2.03	0.41
1:A:409:ARG:O	1:A:410:ALA:HB3	2.21	0.41
2:E:193:G:H2'	2:E:194:C:C6	2.56	0.40
1:B:331:LEU:HB3	1:B:389:HIS:NE2	2.36	0.40
1:A:477:TRP:HH2	1:A:508:LEU:HB3	1.85	0.40
2:E:209:C:O2'	2:E:210:U:P	2.80	0.40
1:B:375:TYR:HA	1:B:378:MET:HG3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:220:C:O2'	2:F:188:C:OP1[8_565]	2.12	0.08

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	
1	A	232/257 (90%)	213 (92%)	18 (8%)	1 (0%)	39	80
1	B	220/257 (86%)	198 (90%)	21 (10%)	1 (0%)	34	76
All	All	452/514 (88%)	411 (91%)	39 (9%)	2 (0%)	39	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	THR
1	B	328	GLY

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	
1	A	207/222 (93%)	178 (86%)	29 (14%)	4	19
1	B	200/222 (90%)	173 (86%)	27 (14%)	5	20
All	All	407/444 (92%)	351 (86%)	56 (14%)	4	20

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	320	LEU
1	A	333	ARG
1	A	337	THR
1	A	342	ARG
1	A	343	ARG
1	A	352	LEU
1	A	356	GLU
1	A	381	VAL
1	A	386	LEU
1	A	396	SER
1	A	398	LEU

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Mol	Chain	Res	Type
1	A	414	GLU
1	A	415	LEU
1	A	418	LEU
1	A	428	VAL
1	A	436	LEU
1	A	444	LEU
1	A	453	GLN
1	A	457	ARG
1	A	462	LEU
1	A	474	GLU
1	A	504	ARG
1	A	508	LEU
1	A	512	LEU
1	A	523	LEU
1	A	552	GLN
1	A	560	ILE
1	A	567	GLU
1	B	317	SER
1	B	320	LEU
1	B	324	ARG
1	B	327	HIS
1	B	331	LEU
1	B	342	ARG
1	B	349	LEU
1	B	352	LEU
1	B	378	MET
1	B	398	LEU
1	B	401	MET
1	B	405	VAL
1	B	407	LEU
1	B	408	SER
1	B	414	GLU
1	B	415	LEU
1	B	437	THR
1	B	456	SER
1	B	457	ARG
1	B	462	LEU
1	B	478	LYS
1	B	488	LYS
1	B	521	VAL
1	B	541	ARG
1	B	544	ARG

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Mol	Chain	Res	Type
1	B	558	ARG
1	B	562	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	545	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	46/51 (90%)	24 (52%)	3 (6%)
2	F	46/51 (90%)	25 (54%)	2 (4%)
All	All	92/102 (90%)	49 (53%)	5 (5%)

All (49) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	171	G
2	E	172	A
2	E	175	G
2	E	176	C
2	E	177	C
2	E	178	G
2	E	182	U
2	E	183	C
2	E	184	A
2	E	185	G
2	E	187	U
2	E	188	C
2	E	189	G
2	E	190	G
2	E	193	G
2	E	198	G
2	E	200	A
2	E	204	U
2	E	210	U
2	E	211	C
2	E	214	U
2	E	215	U

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Mol	Chain	Res	Type
2	E	216	G
2	E	217	U
2	F	175	G
2	F	176	C
2	F	177	C
2	F	178	G
2	F	182	U
2	F	183	C
2	F	184	A
2	F	185	G
2	F	187	U
2	F	188	C
2	F	189	G
2	F	190	G
2	F	191	C
2	F	193	G
2	F	199	A
2	F	200	A
2	F	203	G
2	F	204	U
2	F	210	U
2	F	211	C
2	F	213	G
2	F	214	U
2	F	215	U
2	F	216	G
2	F	217	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	187	U
2	E	209	C
2	E	210	U
2	F	209	C
2	F	210	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
3	SO4	A	601	-	4,4,4	0.32	0	6,6,6	0.16	0
3	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	A	603	-	4,4,4	0.27	0	6,6,6	0.25	0
3	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	A	605	-	4,4,4	0.22	0	6,6,6	0.13	0
3	SO4	A	606	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	A	607	-	4,4,4	0.09	0	6,6,6	0.24	0
3	SO4	A	608	-	4,4,4	0.20	0	6,6,6	0.31	0
3	SO4	B	601	-	4,4,4	0.34	0	6,6,6	0.26	0
3	SO4	B	602	-	4,4,4	0.21	0	6,6,6	0.19	0
3	SO4	B	603	-	4,4,4	0.30	0	6,6,6	0.21	0
3	SO4	B	604	-	4,4,4	0.25	0	6,6,6	0.07	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
3	SO4	A	601	-	-	0/0/0/0	0/0/0/0
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
3	SO4	A	606	-	-	0/0/0/0	0/0/0/0
3	SO4	A	607	-	-	0/0/0/0	0/0/0/0
3	SO4	A	608	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	601	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	SO4	3	0
3	A	607	SO4	1	0
3	B	603	SO4	1	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	A	240/257 (93%)	-0.24	1 (0%) 93 80	35, 57, 127, 157	0
1	B	228/257 (88%)	0.02	8 (3%) 48 21	48, 84, 139, 187	0
2	E	47/51 (92%)	0.21	2 (4%) 39 16	80, 111, 200, 228	0
2	F	47/51 (92%)	1.13	10 (21%) 1 1	114, 157, 275, 331	0
All	All	562/616 (91%)	0.02	21 (3%) 45 19	35, 79, 164, 331	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	170	G	7.0
2	F	171	G	6.5
2	F	218	U	6.1
1	B	339	ALA	5.8
2	F	172	A	4.7
1	B	340	GLY	4.4
2	F	219	C	4.3
2	E	187	U	4.2
2	F	215	U	4.2
1	B	337	THR	3.4
1	B	410	ALA	3.2
2	E	175	G	3.1
2	F	220	C	3.0
1	B	338	ALA	2.6
1	B	341	PRO	2.5
2	F	200	A	2.4
2	F	217	U	2.4
2	F	216	G	2.3
1	B	335	ARG	2.2
1	A	533	SER	2.1
1	B	409	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
3	SO4	A	608	5/5	0.89	0.43	5.60	97,117,121,138	0
3	SO4	A	603	5/5	0.96	0.29	4.61	95,96,109,135	0
3	SO4	A	604	5/5	0.98	0.17	-0.76	61,75,81,83	0
3	SO4	B	601	5/5	0.99	0.13	-1.89	55,69,84,90	0
3	SO4	B	603	5/5	0.97	0.11	-2.35	70,84,93,97	0
3	SO4	A	607	5/5	0.98	0.13	-2.61	56,65,72,75	0
3	SO4	A	606	5/5	0.99	0.11	-3.32	80,86,92,97	0
3	SO4	A	602	5/5	0.94	0.13	-	115,120,122,130	0
3	SO4	B	604	5/5	0.94	0.28	-	138,138,146,147	0
3	SO4	A	605	5/5	0.90	0.18	-	139,146,154,155	0
3	SO4	A	601	5/5	0.99	0.30	-	42,43,65,76	5
3	SO4	B	602	5/5	0.89	0.25	-	113,129,136,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.