Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:23 AM GMT

PDB ID : 1H4S
Title : PROLYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS COMPLEXED WITH TRNAPRO(CGG) AND A PROLYL-ADENYLATE ANALOGUE
Authors : Yaremchuk, A.; Tukalo, M.; Cusack, S.
Deposited on : 2001-05-14
Resolution : 2.85 Å(reported)

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

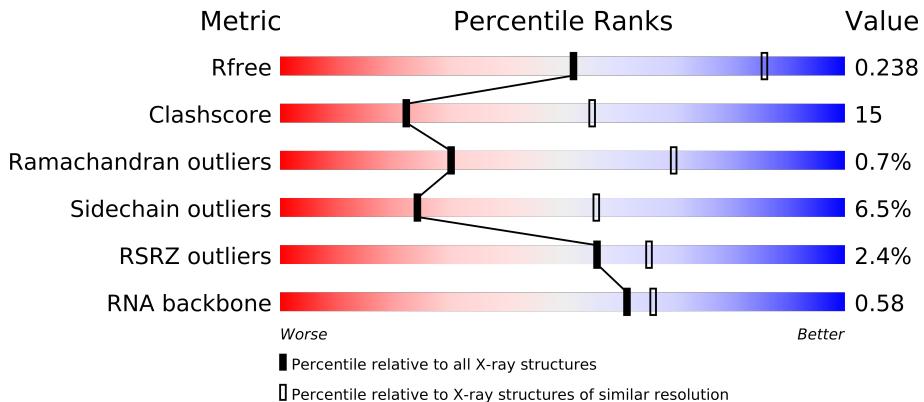|		
MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.85 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		0.238
Clashscore		15
Ramachandran outliers		0.7%
Sidechain outliers		6.5%
RSRZ outliers		2.4%
RNA backbone		0.58

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}	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)
RNA backbone	1838	1014 (3.32-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	477	
1	B	477	
2	T	77	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9192 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROLYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total 3820	C 2442	N 671	O 695	S 12	81	0	0
1	B	473	Total 3820	C 2442	N 671	O 695	S 12	72	0	0
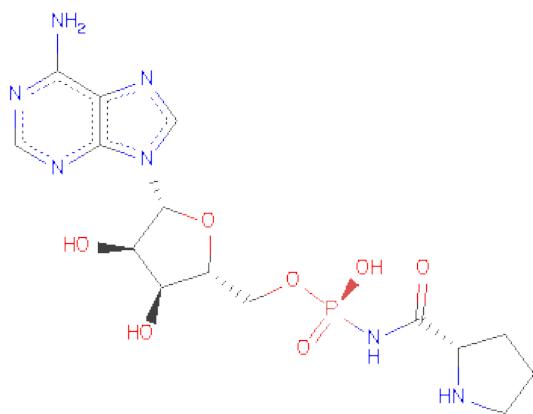
- Molecule 2 is a RNA chain called TRNAPRO(CGG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	67	Total 1439	C 640	N 262	O 470	P 67	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).
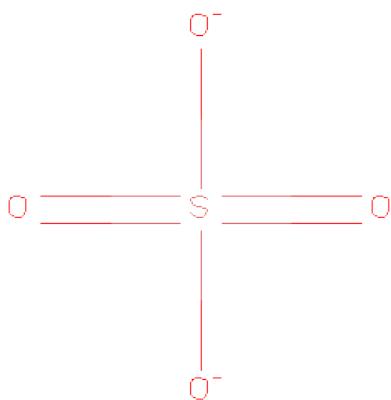
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0

- Molecule 4 is 5'-O-[N-(PROLYL)-SULFAMOYL]ADENOSINE (three-letter code: PSD) (formula: $C_{15}H_{22}N_7O_7P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 15	N 7	O 7	P 1	0	0
4	B	1	Total 29	C 15	N 7	O 7		0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

• Molecule 6 is water.
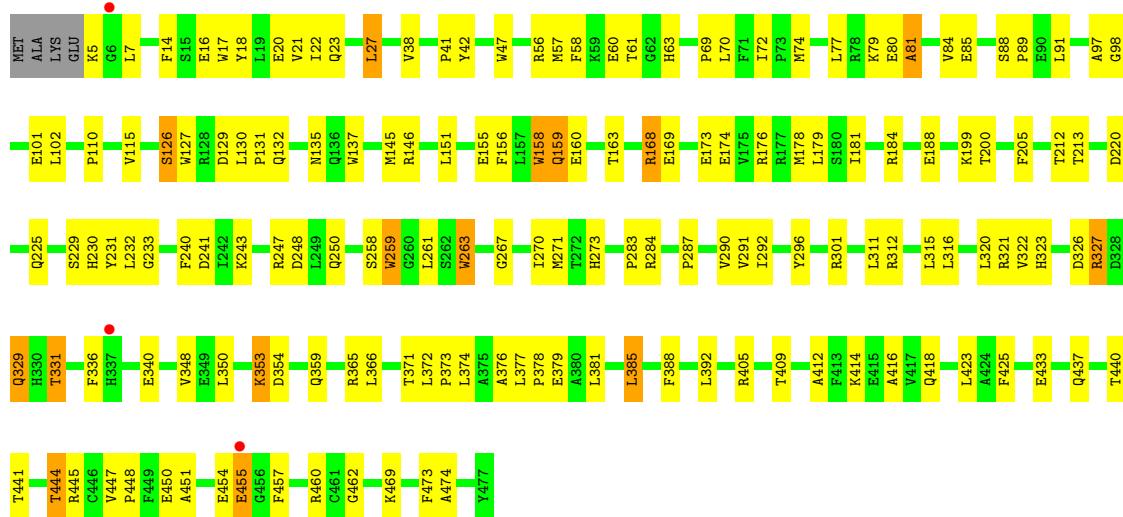
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total 23	O 23	0	0
6	B	7	Total 7	O 7	0	0
6	T	2	Total 2	O 2	0	0

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3 Residue-property plots ⓘ

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 d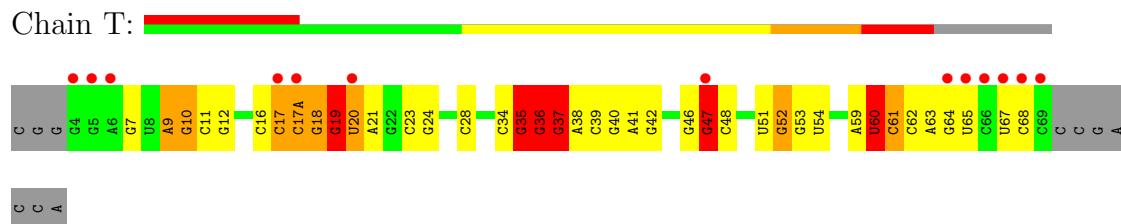isplayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or 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: PROLYL-TRNA SYNTHETASE

Chain A:

- Molecule 1: PROLYL-TRNA SYNTHETASE

Chain B:

- Molecule 2: TRNAPRO(CGG)

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.78Å 140.78Å 236.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 19.94 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.85) 98.0 (19.94-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.58 (at 2.83Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.210 , 0.242 0.205 , 0.238	Depositor DCC
R_{free} test set	2797 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.50$, $<L^2> = 0.34$	Xtriage
Outliers	0 of 54988 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9192	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, SO4, PSD, PSU

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	0/3919	0.64	0/5308
1	B	0.38	0/3919	0.63	0/5308
2	T	0.48	0/1563	0.92	9/2438 (0.4%)
All	All	0.41	0/9401	0.70	9/13054 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	35	G	N9-C1'-C2'	7.81	124.16	114.00
2	T	19	G	N9-C1'-C2'	6.67	122.67	114.00
2	T	37	G	N9-C1'-C2'	6.61	122.59	114.00
2	T	47	G	N9-C1'-C2'	5.75	121.47	114.00
2	T	60	U	C5'-C4'-C3'	-5.68	106.91	116.00
2	T	36	G	N9-C1'-C2'	5.44	121.07	114.00
2	T	48	C	O4'-C1'-N1	5.32	112.45	108.20
2	T	47	G	O4'-C1'-N9	5.05	112.24	108.20
2	T	48	C	N1-C1'-C2'	5.02	120.53	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts (i)

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3820	0	3749	123	0
1	B	3820	0	3749	115	0
2	T	1439	0	729	28	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	21	3	0
4	B	29	0	20	2	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	23	0	0	1	0
6	B	7	0	0	0	0
6	T	2	0	0	0	0
All	All	9192	0	8268	254	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (254) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:120:TRP:NE1	1:B:132:GLN:HG2	1.72	1.05
1:A:168:ARG:HB3	1:A:168:ARG:HH11	1.24	0.97
1:B:120:TRP:HE1	1:B:132:GLN:HG2	1.39	0.87
1:B:448:PRO:HG2	1:B:451:ALA:HB2	1.57	0.86
1:A:329:GLN:HG2	1:B:128:ARG:NH2	1.95	0.81
1:A:77:LEU:O	1:A:84:VAL:HB	1.80	0.81
1:B:77:LEU:O	1:B:84:VAL:HB	1.81	0.80
2:T:18:G:O2'	2:T:19:G:H5'	1.83	0.79
1:B:58:PHE:HE2	1:B:159:GLN:HG3	1.50	0.76
1:A:232:LEU:HD11	1:A:258:SER:HB2	1.68	0.75
1:A:329:GLN:HG2	1:B:128:ARG:CZ	2.18	0.74
1:B:232:LEU:HD11	1:B:258:SER:HB2	1.69	0.73
1:A:56:ARG:O	1:A:60:GLU:HG3	1.92	0.69
1:A:448:PRO:HG2	1:A:451:ALA:HB2	1.74	0.69
1:A:58:PHE:HE2	1:A:159:GLN:HG3	1.56	0.69
1:B:289:GLN:HG3	1:B:321:ARG:HB2	1.75	0.69
1:A:283:PRO:HB3	1:A:385:LEU:HD12	1.74	0.68
1:B:74:MET:HE1	1:B:77:LEU:HD12	1.75	0.68
2:T:51:U:H2'	2:T:52:G:O4'	1.94	0.67
1:B:120:TRP:CE2	1:B:132:GLN:HG2	2.28	0.67
1:A:409:THR:HG23	1:A:412:ALA:H	1.59	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:97:ALA:HB3	1:B:102:LEU:HD21	1.78	0.66
1:A:126:SER:HB2	2:T:28:C:H5'	1.77	0.66
1:A:74:MET:HE1	1:A:77:LEU:HD12	1.78	0.66
2:T:67:U:H2'	2:T:68:C:C6	2.31	0.65
1:A:81:ALA:O	1:A:85:GLU:HG3	1.96	0.65
1:A:97:ALA:HB3	1:A:102:LEU:HD21	1.79	0.65
1:B:238:ARG:HG2	1:B:253:TYR:CE1	2.32	0.65
1:A:168:ARG:CB	1:A:168:ARG:HH11	2.04	0.65
1:B:179:LEU:HD22	1:B:212:THR:HB	1.78	0.64
1:A:336:PHE:O	1:A:340:GLU:HG3	1.98	0.64
1:A:179:LEU:HD22	1:A:212:THR:HB	1.79	0.63
1:B:72:ILE:HG12	1:B:115:VAL:HG21	1.80	0.63
1:A:72:ILE:HG12	1:A:115:VAL:HG21	1.80	0.63
1:A:72:ILE:HG12	1:A:115:VAL:CG2	2.30	0.62
1:B:120:TRP:HE1	1:B:132:GLN:CG	2.11	0.62
1:B:351:GLY:HA3	2:T:35:G:C6	2.34	0.62
1:B:56:ARG:O	1:B:60:GLU:HG3	1.99	0.62
1:B:305:LEU:O	1:B:309:GLN:HG3	1.99	0.62
1:A:290:VAL:HG21	1:A:381:LEU:HD13	1.82	0.61
1:A:451:ALA:HB3	1:A:469:LYS:HD3	1.82	0.61
1:B:72:ILE:HG12	1:B:115:VAL:CG2	2.30	0.61
1:B:414:LYS:O	1:B:418:GLN:HG2	2.02	0.60
1:B:168:ARG:O	1:B:172:GLU:HG3	2.02	0.60
1:B:243:LYS:HE2	1:B:253:TYR:CE2	2.37	0.59
1:B:451:ALA:HB3	1:B:469:LYS:HD3	1.83	0.59
1:B:53:VAL:HA	1:B:56:ARG:NH1	2.18	0.59
1:B:313:GLN:NE2	1:B:313:GLN:HA	2.17	0.59
1:A:248:ASP:OD2	1:A:250:GLN:HB2	2.03	0.59
1:A:259:TRP:C	4:A:1478:PSD:HCG1	2.23	0.58
1:A:290:VAL:HG21	1:A:381:LEU:CD1	2.32	0.58
1:B:283:PRO:HB3	1:B:385:LEU:HD12	1.86	0.58
1:B:373:PRO:HG2	1:B:376:ALA:CB	2.34	0.58
2:T:20:U:H4'	2:T:21:A:H5'	1.85	0.58
1:A:84:VAL:O	1:A:88:SER:HB2	2.03	0.58
2:T:64:G:H2'	2:T:65:U:C6	2.39	0.58
1:A:353:LYS:NZ	1:A:353:LYS:HB3	2.19	0.57
1:B:372:LEU:HD12	1:B:377:LEU:CD1	2.34	0.57
1:B:371:THR:O	1:B:372:LEU:HD23	2.04	0.57
1:B:448:PRO:CG	1:B:451:ALA:HB2	2.33	0.57
1:B:199:LYS:HE2	1:B:213:THR:HG21	1.87	0.56
1:B:84:VAL:O	1:B:88:SER:HB2	2.05	0.56
1:A:373:PRO:HG2	1:A:376:ALA:CB	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:243:LYS:HG2	1:B:253:TYR:CE2	2.41	0.56
1:A:42:TYR:CE2	1:A:287:PRO:HG2	2.41	0.56
1:A:457:PHE:HB3	1:A:462:GLY:O	2.06	0.56
1:A:365:ARG:HG3	1:A:365:ARG:O	2.06	0.55
1:B:349:GLU:HB2	1:B:361:VAL:HB	1.87	0.55
1:A:126:SER:O	1:A:129:ASP:HB2	2.05	0.55
1:B:200:THR:HG23	1:B:444:THR:HG21	1.89	0.54
2:T:23:C:H2'	2:T:24:G:H8	1.72	0.54
1:B:409:THR:HG23	1:B:412:ALA:HB2	1.89	0.54
1:B:79:LYS:HD2	1:B:240:PHE:CE1	2.42	0.54
1:A:199:LYS:HE2	1:A:213:THR:HG21	1.90	0.54
2:T:17(A):C:H5"	2:T:18:G:OP2	2.07	0.54
1:B:373:PRO:HG2	1:B:376:ALA:HB3	1.90	0.54
1:B:366:LEU:HD22	1:B:388:PHE:CE1	2.43	0.54
1:B:53:VAL:HA	1:B:56:ARG:HH12	1.72	0.54
1:B:377:LEU:HB3	1:B:378:PRO:HD3	1.90	0.54
1:A:126:SER:HB2	2:T:28:C:C5'	2.37	0.53
1:A:433:GLU:OE2	1:A:444:THR:HB	2.09	0.53
1:B:313:GLN:HE21	1:B:313:GLN:HA	1.74	0.53
1:A:322:VAL:HG22	1:A:323:HIS:N	2.24	0.52
1:A:160:GLU:HB2	4:A:1478:PSD:HCD2	1.90	0.52
1:A:283:PRO:HG3	1:A:388:PHE:CD2	2.44	0.52
1:A:137:TRP:CZ3	1:A:159:GLN:HB2	2.45	0.52
1:B:137:TRP:CZ3	1:B:159:GLN:HB2	2.45	0.52
1:B:324:LEU:HG	1:B:326:ASP:OD1	2.10	0.52
1:B:290:VAL:HG21	1:B:381:LEU:HD13	1.92	0.52
1:A:155:GLU:OE2	1:B:70:LEU:HB2	2.10	0.52
1:A:151:LEU:HD21	1:A:271:MET:HE1	1.90	0.52
1:A:200:THR:HG23	1:A:444:THR:HG21	1.92	0.52
1:B:205:PHE:HB2	1:B:230:HIS:CE1	2.44	0.51
1:A:130:LEU:HB3	1:A:131:PRO:HA	1.92	0.51
1:A:205:PHE:HB2	1:A:230:HIS:CE1	2.46	0.51
1:B:425:PHE:HZ	1:B:454:GLU:HB3	1.76	0.51
1:B:338:GLU:O	1:B:341:LEU:HB3	2.10	0.51
1:B:151:LEU:HD21	1:B:271:MET:HE1	1.91	0.51
1:A:58:PHE:CE2	1:A:159:GLN:HG3	2.42	0.51
1:A:70:LEU:HB2	1:B:155:GLU:OE2	2.10	0.51
1:B:409:THR:HG23	1:B:412:ALA:CB	2.41	0.51
1:A:127:TRP:CE2	1:A:247:ARG:HG2	2.46	0.51
2:T:52:G:O6	2:T:62:C:N3	2.44	0.50
2:T:23:C:H2'	2:T:24:G:C8	2.45	0.50
1:A:79:LYS:HD2	1:A:240:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:370:GLU:OE1	1:B:372:LEU:HD21	2.10	0.50
1:A:326:ASP:O	1:A:327:ARG:C	2.50	0.50
1:A:88:SER:HB3	1:A:89:PRO:HD3	1.92	0.50
1:B:158:TRP:C	1:B:158:TRP:CD1	2.83	0.50
2:T:17(A):C:H4'	2:T:18:G:OP1	2.12	0.50
1:A:14:PHE:CG	1:A:220:ASP:HB3	2.47	0.50
1:A:241:ASP:OD1	1:A:243:LYS:HE3	2.12	0.49
1:A:158:TRP:C	1:A:158:TRP:CD1	2.85	0.49
1:A:315:LEU:HD22	1:A:320:LEU:HD12	1.95	0.49
1:A:414:LYS:O	1:A:418:GLN:HG2	2.11	0.49
1:A:448:PRO:CG	1:A:451:ALA:HB2	2.41	0.49
1:B:243:LYS:HG2	1:B:253:TYR:CD2	2.46	0.49
1:B:14:PHE:CG	1:B:220:ASP:HB3	2.47	0.49
1:A:273:HIS:ND1	1:A:392:LEU:HD22	2.27	0.49
4:B:1478:PSD:N10	4:B:1478:PSD:O1P	2.45	0.49
1:B:88:SER:HB3	1:B:89:PRO:HD3	1.93	0.49
2:T:17:C:H2'	2:T:17(A):C:H5	1.77	0.49
1:B:241:ASP:OD1	1:B:243:LYS:HE3	2.13	0.49
1:B:132:GLN:O	1:B:163:THR:HA	2.12	0.48
1:A:168:ARG:HG3	1:A:231:TYR:OH	2.13	0.48
1:B:284:ARG:NH1	1:B:389:HIS:CD2	2.80	0.48
1:A:373:PRO:HG2	1:A:376:ALA:HB2	1.94	0.48
1:A:322:VAL:CG2	1:A:323:HIS:N	2.76	0.48
1:A:169:GLU:O	1:A:173:GLU:HG3	2.14	0.48
1:A:377:LEU:HB3	1:A:378:PRO:HD3	1.95	0.47
1:A:151:LEU:HD21	1:A:271:MET:CE	2.45	0.47
2:T:67:U:H2'	2:T:68:C:H6	1.76	0.47
1:A:89:PRO:O	1:B:98:GLY:HA2	2.14	0.47
1:B:169:GLU:O	1:B:173:GLU:HG3	2.15	0.47
1:A:329:GLN:CD	1:A:329:GLN:H	2.17	0.47
1:B:200:THR:CG2	1:B:444:THR:HG21	2.45	0.47
1:B:445:ARG:HA	1:B:445:ARG:NE	2.29	0.47
1:B:178:MET:HG3	1:B:259:TRP:CE2	2.50	0.47
1:B:74:MET:CE	1:B:77:LEU:HD12	2.45	0.47
1:B:435:LEU:O	1:B:439:GLU:HG3	2.15	0.47
1:A:371:THR:O	1:A:372:LEU:HD23	2.14	0.47
2:T:17:C:H2'	2:T:17(A):C:C5	2.50	0.46
1:A:445:ARG:HA	1:A:445:ARG:NE	2.31	0.46
1:B:354:ASP:CG	2:T:35:G:H1	2.19	0.46
1:A:261:LEU:C	1:A:261:LEU:HD23	2.36	0.46
1:B:425:PHE:CZ	1:B:454:GLU:HB3	2.50	0.46
1:B:366:LEU:HD12	1:B:366:LEU:HA	1.76	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:312:ARG:NH1	1:A:316:LEU:HD11	2.31	0.46
1:A:405:ARG:HD3	1:A:416:ALA:HB2	1.98	0.46
1:B:454:GLU:OE1	1:B:470:ARG:HD2	2.16	0.46
1:B:18:TYR:O	1:B:21:VAL:HG12	2.16	0.46
1:A:178:MET:HG3	1:A:259:TRP:CE2	2.51	0.45
2:T:60:U:H5"	2:T:61:C:H5	1.81	0.45
1:A:321:ARG:HG3	1:A:321:ARG:HH11	1.81	0.45
2:T:40:G:H2'	2:T:41:A:C8	2.51	0.45
1:A:57:MET:HE3	1:A:181:ILE:HG23	1.98	0.45
1:A:18:TYR:CZ	1:A:22:ILE:HD11	2.51	0.45
2:T:64:G:H2'	2:T:65:U:H6	1.80	0.45
2:T:11:C:O2'	2:T:12:G:H5'	2.17	0.45
1:B:151:LEU:CD1	1:B:267:GLY:HA3	2.47	0.45
1:B:137:TRP:CE3	1:B:159:GLN:HB2	2.51	0.45
1:B:184:ARG:HG3	1:B:188:GLU:OE2	2.16	0.45
2:T:46:G:H3'	2:T:47:G:H21	1.81	0.45
1:B:27:LEU:HD23	1:B:270:ILE:HD11	1.98	0.45
1:A:151:LEU:CD1	1:A:267:GLY:HA3	2.47	0.45
1:B:18:TYR:CZ	1:B:22:ILE:HD11	2.52	0.45
1:A:137:TRP:CE3	1:A:159:GLN:HB2	2.52	0.45
2:T:41:A:H2'	2:T:42:G:O4'	2.18	0.44
1:B:411:GLU:O	1:B:415:GLU:HG3	2.16	0.44
2:T:9:A:H4'	2:T:10:G:OP1	2.17	0.44
2:T:36:G:H4'	2:T:37:G:O5'	2.18	0.44
1:A:473:PHE:O	1:A:474:ALA:HB2	2.18	0.44
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.81	0.44
1:A:18:TYR:O	1:A:21:VAL:HG12	2.18	0.44
1:A:158:TRP:CZ3	4:A:1478:PSD:H5'1	2.53	0.44
1:B:282:PRO:HA	1:B:283:PRO:HD3	1.83	0.44
1:B:315:LEU:HD21	1:B:381:LEU:HD12	2.00	0.44
1:A:437:GLN:O	1:A:441:THR:HA	2.16	0.44
1:A:74:MET:HE1	1:A:91:LEU:HD13	1.99	0.44
1:B:135:ASN:OD1	1:B:159:GLN:HG2	2.18	0.44
1:A:38:VAL:HG22	1:B:69:PRO:HD3	2.00	0.44
1:B:457:PHE:HB3	1:B:462:GLY:O	2.18	0.44
1:A:74:MET:CE	1:A:77:LEU:HD12	2.46	0.44
1:A:373:PRO:HG2	1:A:376:ALA:HB3	1.99	0.43
1:B:473:PHE:O	1:B:474:ALA:HB2	2.17	0.43
1:A:14:PHE:CD2	1:A:220:ASP:HB3	2.53	0.43
2:T:53:G:H3'	2:T:54:5MU:H71	2.00	0.43
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.84	0.43
1:B:163:THR:HG21	1:B:174:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:1478:PSD:N10	4:B:1478:PSD:O2P	2.52	0.43
1:A:425:PHE:CZ	1:A:454:GLU:HB3	2.54	0.43
1:B:261:LEU:HD23	1:B:261:LEU:C	2.39	0.43
1:A:291:VAL:O	1:A:291:VAL:HG13	2.17	0.43
1:A:331:THR:HG21	6:A:2019:HOH:O	2.17	0.43
1:A:292:ILE:HD13	1:A:311:LEU:HD23	1.99	0.43
1:B:448:PRO:HG2	1:B:451:ALA:CB	2.36	0.43
1:A:163:THR:HG21	1:A:174:GLU:OE1	2.19	0.43
1:A:200:THR:CG2	1:A:444:THR:HG21	2.48	0.43
1:A:16:GLU:O	1:A:20:GLU:HG3	2.19	0.43
1:B:171:ALA:O	1:B:175:VAL:HG23	2.19	0.43
1:B:74:MET:HE1	1:B:91:LEU:HD13	2.00	0.42
1:B:61:THR:HG1	1:B:63:HIS:CE1	2.37	0.42
1:B:214:ILE:O	1:B:214:ILE:HG13	2.18	0.42
1:A:176:ARG:HD2	1:A:176:ARG:HA	1.77	0.42
1:A:27:LEU:HD23	1:A:270:ILE:HD11	2.02	0.42
1:A:377:LEU:CB	1:A:378:PRO:HD3	2.49	0.42
1:A:372:LEU:HD12	1:A:377:LEU:HD12	2.01	0.42
1:A:354:ASP:HB3	1:A:359:GLN:O	2.20	0.42
1:A:184:ARG:HG3	1:A:188:GLU:OE2	2.19	0.42
1:B:151:LEU:HD21	1:B:271:MET:CE	2.49	0.42
1:B:14:PHE:CD2	1:B:220:ASP:HB3	2.54	0.42
1:A:425:PHE:HZ	1:A:454:GLU:HB3	1.84	0.42
1:A:440:THR:C	1:A:441:THR:HG23	2.40	0.42
1:B:336:PHE:O	1:B:340:GLU:HG3	2.19	0.42
1:B:445:ARG:O	1:B:446:CYS:HB3	2.19	0.42
1:B:455:GLU:OE1	1:B:468:GLY:HA2	2.18	0.42
1:B:413:PHE:C	1:B:413:PHE:CD1	2.93	0.42
1:A:301:ARG:NH1	1:A:301:ARG:HG2	2.34	0.42
1:B:65:ASN:HA	1:B:135:ASN:O	2.20	0.42
1:B:399:PHE:O	1:B:403:HIS:HD2	2.02	0.42
1:A:69:PRO:HD3	1:B:38:VAL:HG22	2.02	0.41
2:T:39:C:H2'	2:T:40:G:C8	2.54	0.41
1:A:101:GLU:HA	1:A:101:GLU:OE1	2.20	0.41
1:A:231:TYR:CZ	1:A:233:GLY:HA2	2.56	0.41
1:A:135:ASN:OD1	1:A:159:GLN:HG2	2.19	0.41
1:A:353:LYS:HZ3	1:A:353:LYS:HB3	1.86	0.41
1:B:161:GLY:HA3	1:B:259:TRP:CE3	2.56	0.41
1:A:311:LEU:HD21	1:A:348:VAL:HG11	2.02	0.41
1:A:98:GLY:HA2	1:B:89:PRO:O	2.21	0.41
1:A:447:VAL:HG12	1:A:469:LYS:HD2	2.01	0.41
1:B:231:TYR:CZ	1:B:233:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:58:PHE:CE2	1:B:159:GLN:HG3	2.41	0.41
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.93	0.41
1:B:161:GLY:HA3	1:B:259:TRP:CZ3	2.56	0.41
1:A:329:GLN:HG2	1:B:128:ARG:HH22	1.82	0.41
1:A:321:ARG:HG3	1:A:321:ARG:NH1	2.36	0.41
1:B:19:LEU:HG	1:B:30:TYR:OH	2.21	0.41
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.71	0.41
1:A:155:GLU:HG2	1:A:156:PHE:N	2.35	0.41
1:B:101:GLU:HA	1:B:101:GLU:OE1	2.22	0.41
1:B:317:ALA:C	1:B:319:GLY:H	2.23	0.41
1:A:47:TRP:CZ3	1:A:263:TRP:HA	2.56	0.41
1:A:212:THR:OG1	1:A:229:SER:HB3	2.21	0.40
1:A:350:LEU:HD21	1:A:374:LEU:HD11	2.03	0.40
1:A:61:THR:HG1	1:A:63:HIS:CE1	2.39	0.40
1:A:329:GLN:HG2	1:B:128:ARG:NH1	2.35	0.40
2:T:63:A:H2'	2:T:64:G:O4'	2.22	0.40
1:A:132:GLN:O	1:A:163:THR:HA	2.21	0.40
1:A:455:GLU:HA	1:A:455:GLU:OE1	2.21	0.40
1:B:373:PRO:HG2	1:B:376:ALA:HB2	2.03	0.40
1:A:7:LEU:HD11	1:A:17:TRP:CD1	2.56	0.40
1:B:90:GLU:HG2	1:B:90:GLU:H	1.73	0.40
1:A:248:ASP:C	1:A:250:GLN:H	2.24	0.40
1:B:140:VAL:HG11	1:B:158:TRP:CZ2	2.56	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	
1	A	471/477 (99%)	439 (93%)	28 (6%)	4 (1%)	27	66
1	B	471/477 (99%)	441 (94%)	27 (6%)	3 (1%)	33	73
All	All	942/954 (99%)	880 (93%)	55 (6%)	7 (1%)	30	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ARG
1	A	146	ARG
1	B	146	ARG
1	A	81	ALA
1	B	81	ALA
1	B	110	PRO
1	A	110	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	
1	A	392/395 (99%)	366 (93%)	26 (7%)	24	55
1	B	392/395 (99%)	367 (94%)	25 (6%)	25	57
All	All	784/790 (99%)	733 (94%)	51 (6%)	24	56

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	23	GLN
1	A	27	LEU
1	A	41	PRO
1	A	80	GLU
1	A	126	SER
1	A	145	MET
1	A	158	TRP
1	A	159	GLN
1	A	168	ARG
1	A	225	GLN
1	A	259	TRP
1	A	263	TRP
1	A	284	ARG
1	A	296	TYR
1	A	329	GLN
1	A	331	THR
1	A	353	LYS
1	A	366	LEU

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Mol	Chain	Res	Type
1	A	379	GLU
1	A	385	LEU
1	A	423	LEU
1	A	444	THR
1	A	450	GLU
1	A	455	GLU
1	A	460	ARG
1	B	23	GLN
1	B	27	LEU
1	B	41	PRO
1	B	80	GLU
1	B	126	SER
1	B	145	MET
1	B	158	TRP
1	B	159	GLN
1	B	225	GLN
1	B	259	TRP
1	B	263	TRP
1	B	299	GLU
1	B	312	ARG
1	B	322	VAL
1	B	329	GLN
1	B	366	LEU
1	B	379	GLU
1	B	385	LEU
1	B	390	GLU
1	B	402	ASP
1	B	409	THR
1	B	423	LEU
1	B	444	THR
1	B	450	GLU
1	B	455	GLU

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	255	HIS
1	B	12	GLN
1	B	96	HIS
1	B	132	GLN
1	B	159	GLN

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Mol	Chain	Res	Type
1	B	255	HIS
1	B	313	GLN
1	B	329	GLN
1	B	359	GLN
1	B	389	HIS
1	B	403	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	T	66/77 (85%)	15 (22%)	7 (10%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	T	9	A
2	T	10	G
2	T	17	C
2	T	17(A)	C
2	T	18	G
2	T	20	U
2	T	35	G
2	T	36	G
2	T	37	G
2	T	38	A
2	T	47	G
2	T	52	G
2	T	59	A
2	T	60	U
2	T	61	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	T	7	G
2	T	9	A
2	T	16	C
2	T	17(A)	C
2	T	19	G
2	T	34	C
2	T	60	U

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

2 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	5MU	T	54	2	20,22,23	0.84	1 (5%)	25,32,35	1.11	5 (20%)
2	PSU	T	55	2	19,21,22	1.16	3 (15%)	23,30,33	1.05	1 (4%)

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	5MU	T	54	2	-	0/6/25/26	0/2/2/2
2	PSU	T	55	2	-	0/8/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	55	PSU	C2-N1	3.11	1.43	1.37
2	T	55	PSU	C6-N1	2.19	1.34	1.32
2	T	54	5MU	C6-C5	-2.12	1.34	1.40
2	T	55	PSU	P-OP1	2.06	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	54	5MU	C6-N1-C2	-2.41	121.72	122.41
2	T	54	5MU	C5M-C5-C6	2.17	123.20	118.59
2	T	55	PSU	C5-C4-N3	-2.15	114.94	118.86
2	T	54	5MU	C5M-C5-C4	-2.15	118.85	121.04
2	T	54	5MU	N3-C2-N1	-2.09	114.23	115.97
2	T	54	5MU	C5-C6-N1	2.08	123.61	121.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	#$|Z| > 2$
4	PSD	A	1478	-	33,33,33	1.08	4 (12%)	49,49,49	1.42	8 (16%)
5	SO4	A	1480	-	4,4,4	0.32	0	6,6,6	0.13	0
5	SO4	A	1481	-	4,4,4	0.25	0	6,6,6	0.09	0
4	PSD	B	1478	-	28,29,33	0.55	0	39,41,49	1.31	6 (15%)
5	SO4	B	1480	-	4,4,4	0.32	0	6,6,6	0.17	0
5	SO4	B	1481	-	4,4,4	0.31	0	6,6,6	0.09	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
4	PSD	A	1478	-	-	0/18/42/42	0/2/4/4
5	SO4	A	1480	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1481	-	-	0/0/0/0	0/0/0/0
4	PSD	B	1478	-	-	0/10/33/42	0/2/4/4
5	SO4	B	1480	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1481	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1478	PSD	C-N10	-3.82	1.33	1.36
4	A	1478	PSD	P-O5'	2.65	1.60	1.57
4	A	1478	PSD	P-O2P	-2.15	1.48	1.55
4	A	1478	PSD	P-O1P	2.04	1.48	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1478	PSD	O2P-P-O1P	4.16	119.48	109.89
4	B	1478	PSD	O4'-C1'-N9	3.29	111.50	108.44
4	A	1478	PSD	O1P-P-N10	-3.24	105.19	111.25
4	A	1478	PSD	O4'-C1'-N9	2.65	110.91	108.44
4	B	1478	PSD	O3'-C3'-C2'	2.42	119.69	111.83
4	A	1478	PSD	O5'-P-N10	2.32	114.96	106.04
4	A	1478	PSD	O2P-P-N10	-2.23	103.45	107.55
4	A	1478	PSD	O3'-C3'-C2'	2.22	119.06	111.83
4	A	1478	PSD	C2'-C3'-C4'	2.22	107.07	102.65
4	B	1478	PSD	C2'-C3'-C4'	2.20	107.04	102.65
4	B	1478	PSD	O4'-C1'-C2'	2.20	110.14	106.77
4	A	1478	PSD	O4'-C1'-C2'	2.10	110.00	106.77
4	B	1478	PSD	O2'-C2'-C1'	-2.03	105.09	111.23
4	B	1478	PSD	C8-N9-C1'	2.02	130.35	126.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	A	472/477 (98%)	-0.20	3 (0%)	86	91	18, 39, 68, 90	18 (3%)
1	B	472/477 (98%)	-0.19	8 (1%)	67	76	19, 41, 67, 85	15 (3%)
2	T	67/77 (87%)	1.01	13 (19%)	2	2	25, 60, 107, 119	0
All	All	1011/1031 (98%)	-0.12	24 (2%)	56	65	18, 41, 73, 119	33 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	5	G	5.7
2	T	4	G	5.7
2	T	69	C	4.6
1	B	6	GLY	3.9
2	T	66	C	3.8
2	T	68	C	3.7
1	B	402	ASP	3.7
2	T	6	A	3.6
2	T	47	G	3.5
2	T	20	U	3.5
2	T	65	U	3.2
2	T	64	G	3.2
1	A	6	GLY	2.9
1	B	249	LEU	2.9
1	B	348	VAL	2.8
2	T	17(A)	C	2.8
2	T	17	C	2.8
2	T	67	U	2.6
1	B	357	GLY	2.2
1	B	292	ILE	2.1
1	A	455	GLU	2.1
1	B	11	SER	2.0
1	B	247	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	337	HIS	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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	PSU	T	55	20/21	0.18	2.11	44,50,54,55	0
2	5MU	T	54	21/22	0.19	1.15	26,45,63,68	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
4	PSD	B	1478	29/30	0.20	0.86	31,41,50,52	0
5	SO4	A	1480	5/5	0.16	-0.44	67,68,70,77	0
5	SO4	B	1480	5/5	0.17	-0.58	72,79,83,89	0
5	SO4	A	1481	5/5	0.15	-0.90	87,89,89,91	0
4	PSD	A	1478	30/30	0.12	-1.30	10,31,39,43	0
3	ZN	B	490	1/1	0.04	-1.93	65,65,65,65	0
5	SO4	B	1481	5/5	0.12	-2.38	74,76,78,78	0
3	ZN	A	490	1/1	0.07	-2.65	50,50,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.