Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 05:23 PM EST

PDB ID	:	4PEI
Title	:	Dbr1 in complex with synthetic branched RNA analog
Authors	:	Montemayor, E.J.; Katolik, A.; Clark, N.E.; Taylor, A.B.; Schuermann, J.P.; Combs, D.J.; Johnsson, R.; Holloway, S.P.; Stevens, S.W.; Damha, M.J.; Hart, P.J.
Deposited on	:	2014-04-23
Resolution	:	1.95 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:

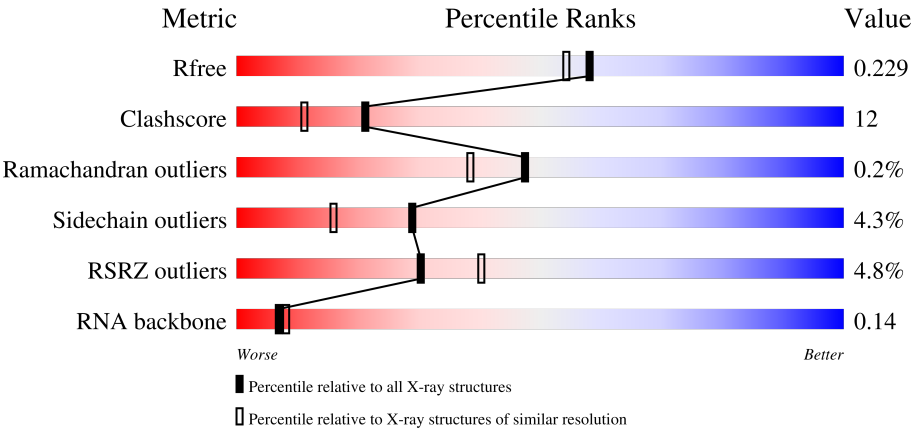
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)
RNA backbone	3102	1124 (2.50-1.42)

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 <=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	356	5% 79% 17%
1	B	356	2% 77% 19%
1	C	356	3% 81% 15%
1	D	356	6% 79% 16%

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Mol	Chain	Length	Quality of chain
1	E	356	6% 72% 24%
2	V	5	20% 40% 20% 40%
2	W	5	20% 40% 20% 40%
2	X	5	20% 40% 40%
2	Y	5	40% 20% 20% 60%
2	Z	5	20% 60% 40%
3	Q	2	50% 50%
3	R	2	50% 50%
3	S	2	50% 50%
3	T	2	50% 50%
3	U	2	50% 50%

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	G46	Q	510	-	-	X	-
3	G46	R	510	-	-	X	-
3	G46	T	510	-	-	X	-
3	G46	U	501	-	-	-	X
7	PG4	B	403	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16230 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 RNA lariat debranching enzyme, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	3	0
			2872	1866	467	525	14			
1	B	349	Total	C	N	O	S	0	3	0
			2876	1869	469	524	14			
1	C	349	Total	C	N	O	S	0	2	0
			2869	1864	466	525	14			
1	D	349	Total	C	N	O	S	0	2	0
			2873	1866	469	524	14			
1	E	348	Total	C	N	O	S	0	3	0
			2875	1867	470	524	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C4M1P9
A	0	ALA	-	expression tag	UNP C4M1P9
A	14	SER	CYS	engineered mutation	UNP C4M1P9
B	-1	GLY	-	expression tag	UNP C4M1P9
B	0	ALA	-	expression tag	UNP C4M1P9
B	14	SER	CYS	engineered mutation	UNP C4M1P9
C	-1	GLY	-	expression tag	UNP C4M1P9
C	0	ALA	-	expression tag	UNP C4M1P9
C	14	SER	CYS	engineered mutation	UNP C4M1P9
D	-1	GLY	-	expression tag	UNP C4M1P9
D	0	ALA	-	expression tag	UNP C4M1P9
D	14	SER	CYS	engineered mutation	UNP C4M1P9
E	-1	GLY	-	expression tag	UNP C4M1P9
E	0	ALA	-	expression tag	UNP C4M1P9
E	14	SER	CYS	engineered mutation	UNP C4M1P9

- Molecule 2 is a RNA chain called RNA (5'-R(*UP*AP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	V	3	Total C N O P 32 14 5 11 2	0	0	0
2	W	3	Total C N O P 32 14 5 11 2	0	0	0
2	X	3	Total C N O P 63 29 13 18 3	0	0	0
2	Y	2	Total C N O P 22 10 5 6 1	0	0	1
2	Z	3	Total C N O P 58 28 13 15 2	0	0	0

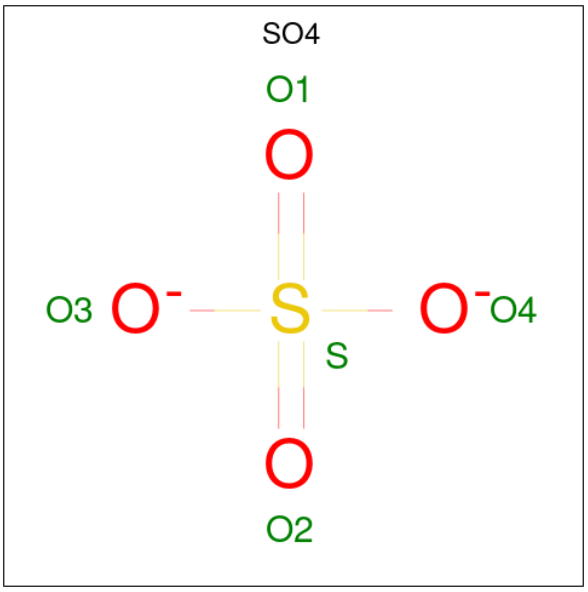
- Molecule 3 is a RNA chain called RNA (5'-R(*(G46)P*U)-3').

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	Q	1	Total C N O P S 24 10 5 7 1 1	0	0	0
3	R	1	Total C O P S 13 5 6 1 1	0	0	0
3	S	1	Total O P S 5 3 1 1	0	0	0
3	T	1	Total O P S 5 3 1 1	0	0	0
3	U	1	Total O 1 1	0	0	1

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

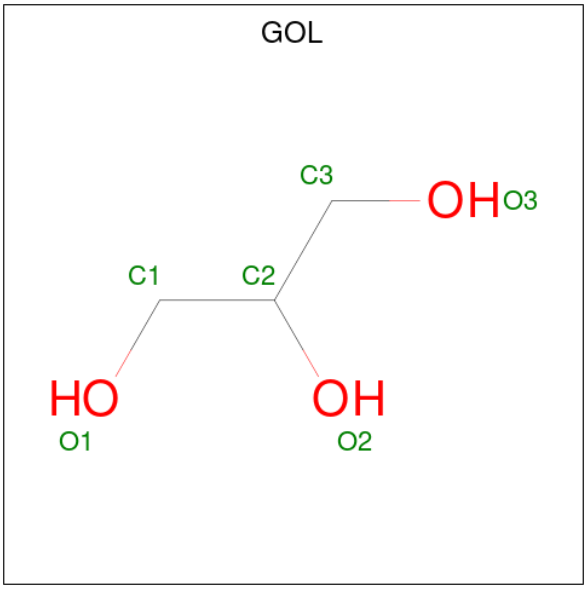
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ni 1 1	0	0
4	B	1	Total Ni 1 1	0	0
4	C	1	Total Ni 1 1	0	0
4	D	1	Total Ni 1 1	0	0
4	E	1	Total Ni 1 1	0	0

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



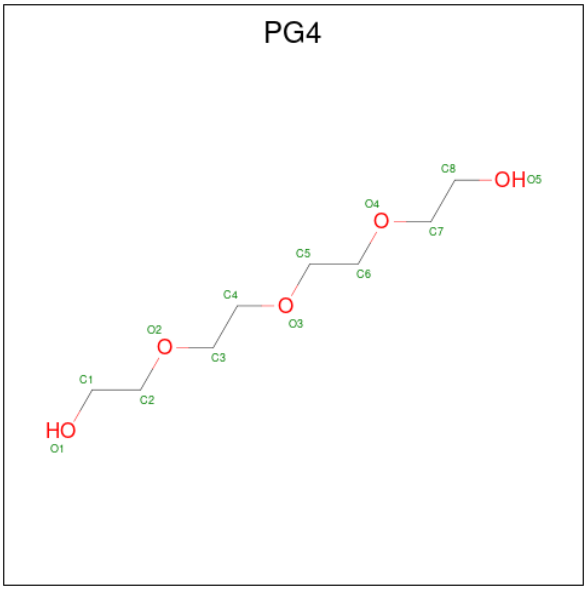
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	338	Total O 338 338	0	0
8	V	3	Total O 3 3	0	0
8	Q	2	Total O 2 2	0	0

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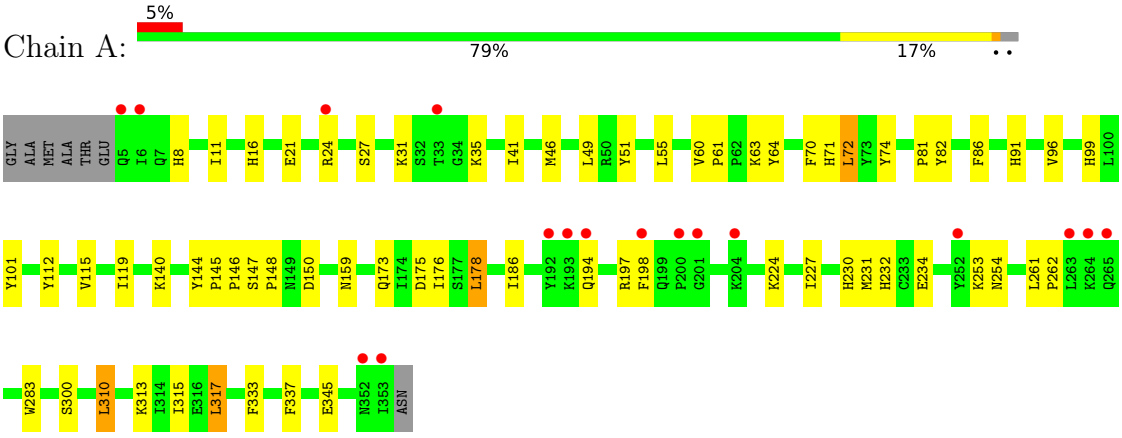
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	271	Total O 271 271	0	0
8	W	2	Total O 2 2	0	0
8	R	1	Total O 1 1	0	0
8	C	325	Total O 325 325	0	0
8	X	5	Total O 5 5	0	0
8	D	301	Total O 301 301	0	0
8	Y	4	Total O 4 4	0	0
8	E	277	Total O 277 277	0	0
8	Z	2	Total O 2 2	0	0

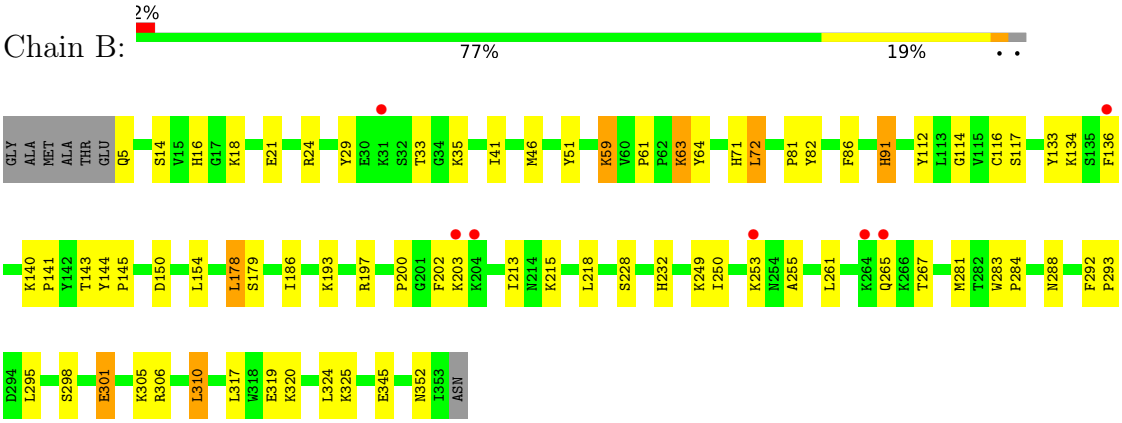
3 Residue-property plots (i)

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.

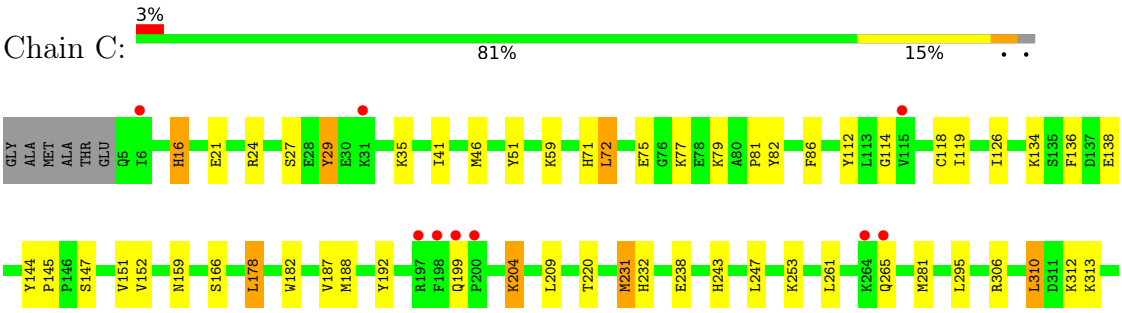
• Molecule 1: RNA lariat debranching enzyme, putative

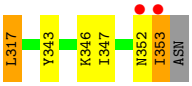


• Molecule 1: RNA lariat debranching enzyme, putative



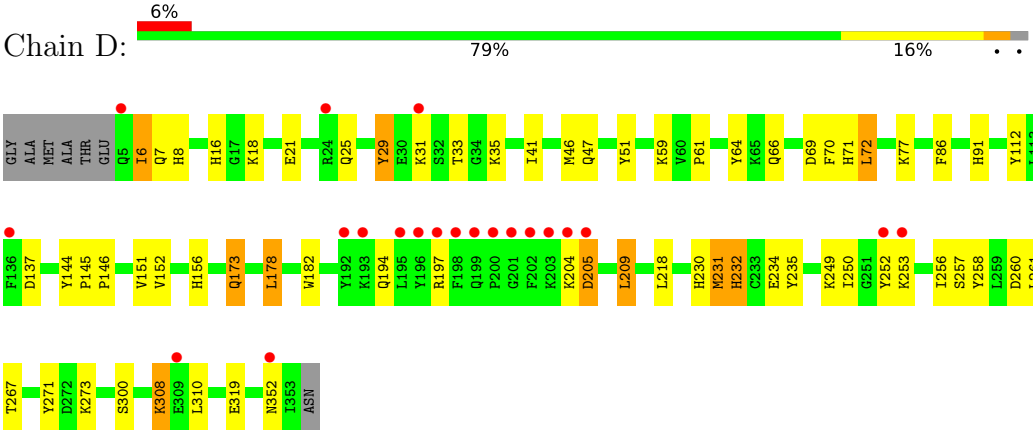
• Molecule 1: RNA lariat debranching enzyme, putative





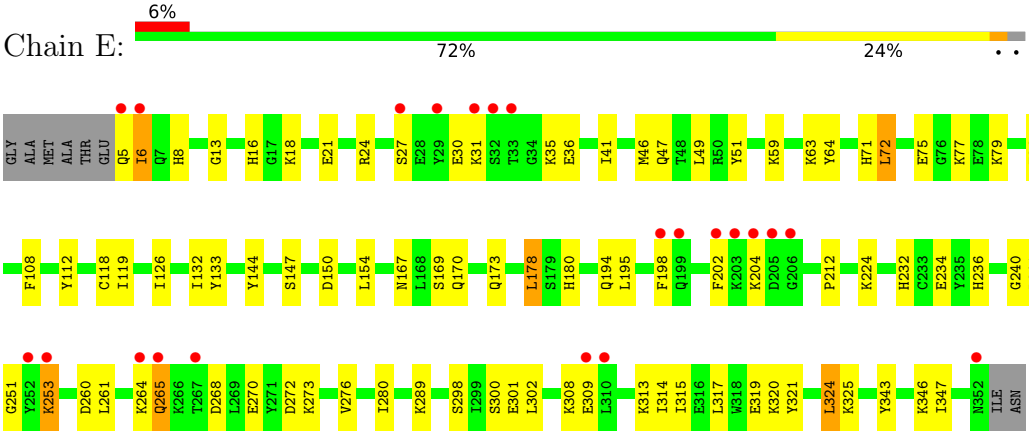
• Molecule 1: RNA lariat debranching enzyme, putative

Chain D:



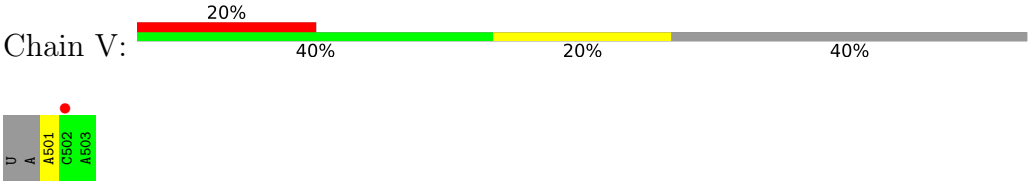
• Molecule 1: RNA lariat debranching enzyme, putative

Chain E:



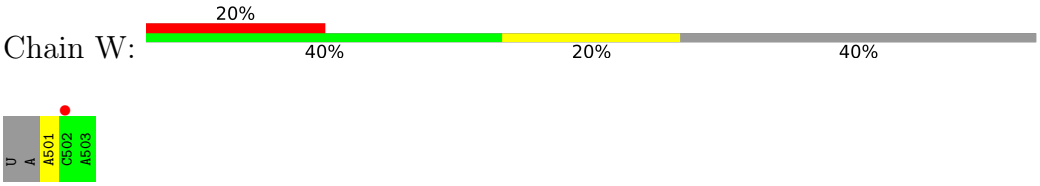
• Molecule 2: RNA (5'-R(*UP*AP*AP*CP*A)-3')

Chain V:



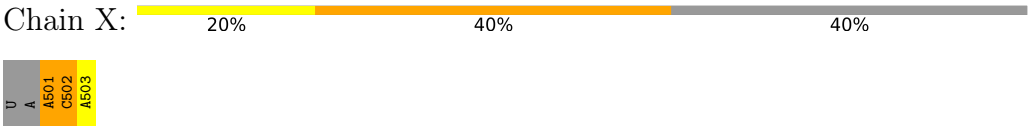
• Molecule 2: RNA (5'-R(*UP*AP*AP*CP*A)-3')

Chain W:



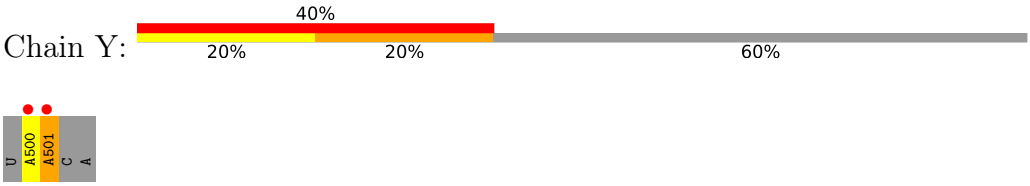
• Molecule 2: RNA (5'-R(*UP*AP*AP*CP*A)-3')

Chain X:



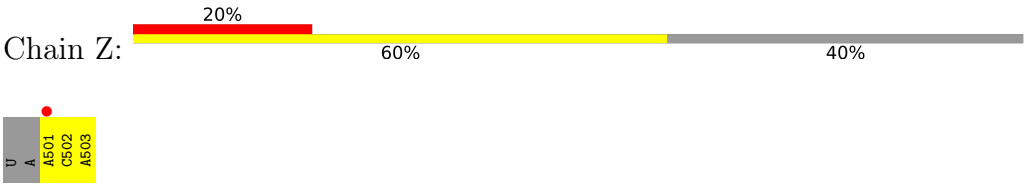
• Molecule 2: RNA (5'-R(*UP*AP*AP*CP*A)-3')

Chain Y:



• Molecule 2: RNA (5'-R(*UP*AP*AP*CP*A)-3')

Chain Z:



• Molecule 3: RNA (5'-R(*(G46)P*U)-3')

Chain Q:

• Molecule 3: RNA (5'-R(*(G46)P*U)-3')

Chain R:

• Molecule 3: RNA (5'-R(*(G46)P*U)-3')

Chain S:

• Molecule 3: RNA (5'-R(*(G46)P*U)-3')

Chain T:

• Molecule 3: RNA (5'-R(*(G46)P*U)-3')

Chain U:


G501
U

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.04Å 142.48Å 214.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.37 – 1.95 46.37 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.37-1.95) 98.8 (46.37-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.184 , 0.229 0.184 , 0.229	Depositor DCC
R_{free} test set	8110 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16230	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, NI, G46, PG4

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	0.68	0/2956	0.71	0/3995
1	B	0.69	1/2961 (0.0%)	0.72	0/4002
1	C	0.72	0/2950	0.73	0/3987
1	D	0.66	0/2952	0.71	0/3990
1	E	0.68	1/2958 (0.0%)	0.72	1/3998 (0.0%)
2	V	0.65	0/35	1.01	0/53
2	W	0.90	0/35	1.15	0/53
2	X	0.63	0/70	1.13	1/106 (0.9%)
2	Y	2.37	1/24 (4.2%)	2.09	2/36 (5.6%)
2	Z	0.53	0/65	0.91	0/99
All	All	0.69	3/15006 (0.0%)	0.73	4/20319 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	500	A	O3'-P	-10.65	1.48	1.61
1	E	241	PRO	N-CD	5.43	1.55	1.47
1	B	91	HIS	C-N	-5.10	1.22	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	501	A	OP1-P-OP2	-8.10	107.45	119.60
2	X	501	A	C4'-C3'-C2'	-5.96	96.64	102.60
2	Y	500	A	OP1-P-O3'	5.57	117.45	105.20
1	E	240	GLY	C-N-CD	5.53	140.01	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2872	0	2846	58	0
1	B	2876	0	2851	73	0
1	C	2869	0	2842	54	0
1	D	2873	0	2842	73	0
1	E	2875	0	2839	83	0
2	V	32	0	14	2	0
2	W	32	0	14	4	0
2	X	63	0	34	3	0
2	Y	22	0	12	17	0
2	Z	58	0	30	13	0
3	Q	24	0	13	7	0
3	R	13	0	8	7	0
3	S	5	0	1	0	0
3	T	5	0	1	7	0
3	U	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	1	0
5	E	5	0	0	0	0
6	A	12	0	16	2	0
6	C	12	0	16	2	0
6	D	12	0	16	1	0
7	B	13	0	18	14	0
8	A	338	0	0	12	0
8	B	271	0	0	9	0
8	C	325	0	0	8	0
8	D	301	0	0	11	0
8	E	277	0	0	7	0
8	Q	2	0	0	0	0
8	R	1	0	0	1	0
8	V	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	W	2	0	0	0	0
8	X	5	0	0	0	0
8	Y	4	0	0	1	0
8	Z	2	0	0	0	0
All	All	16230	0	14413	352	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 12.

All (352) 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:E:91[B]:HIS:NE2	2:Z:502:C:O2'	1.57	1.38
1:D:91:HIS:CE1	2:Y:501:A:H1'	1.62	1.34
1:E:91[B]:HIS:CE1	2:Z:502:C:O2'	1.91	1.24
1:B:143:THR:HG23	7:B:403:PG4:H41	1.24	1.17
1:B:16[B]:HIS:NE2	3:R:510:G46:S2P	2.20	1.13
1:E:173:GLN:NE2	1:E:224:LYS:HE3	1.64	1.11
1:B:141:PRO:HD2	7:B:403:PG4:H51	1.32	1.10
1:E:91[B]:HIS:HE1	8:E:771:HOH:O	1.35	1.08
2:Y:501:A:OP1	2:Y:501:A:H3'	1.54	1.05
1:E:173:GLN:HE22	1:E:224:LYS:HE3	1.20	1.03
1:D:16[A]:HIS:CE1	3:T:510:G46:S2P	2.51	1.02
2:Y:501:A:C8	2:Y:501:A:H5'	1.94	1.01
1:D:91:HIS:HE1	2:Y:501:A:H1'	1.23	1.00
1:C:209:LEU:HD21	1:C:231:MET:CE	1.92	0.99
1:C:192:TYR:CZ	6:C:404:GOL:H12	1.98	0.99
1:C:209:LEU:HD21	1:C:231:MET:HE2	1.45	0.94
1:D:91:HIS:CE1	2:Y:501:A:C1'	2.51	0.94
1:B:16[B]:HIS:HE2	3:R:510:G46:HS	1.12	0.93
1:D:16[A]:HIS:HD2	2:Y:501:A:C2	1.85	0.93
1:B:143:THR:CG2	7:B:403:PG4:H41	2.00	0.91
1:A:173:GLN:NE2	1:A:224:LYS:HE2	1.84	0.90
1:D:91:HIS:CE1	3:T:510:G46:O3P	2.25	0.90
1:E:91[B]:HIS:CD2	2:Z:502:C:O2'	2.26	0.88
1:B:141:PRO:CD	7:B:403:PG4:H51	2.04	0.88
3:R:510:G46:S2P	8:R:601:HOH:O	2.32	0.87
1:E:91[B]:HIS:HE2	2:Z:502:C:C3'	1.88	0.86
1:D:91:HIS:HE1	3:T:510:G46:O3P	1.56	0.86
1:E:91[B]:HIS:NE2	2:Z:502:C:C2'	2.38	0.86
1:B:143:THR:O	7:B:403:PG4:H12	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:NE2	1:A:224:LYS:CE	2.42	0.83
1:C:313:LYS:O	1:C:317:LEU:HD22	1.79	0.83
2:Y:501:A:H5'	2:Y:501:A:H8	1.44	0.81
1:C:192:TYR:CE2	6:C:404:GOL:H12	2.14	0.81
1:D:16[A]:HIS:HE1	3:T:510:G46:S2P	2.01	0.81
1:D:91:HIS:HE1	2:Y:501:A:C1'	1.89	0.80
1:E:173:GLN:CD	1:E:224:LYS:HE3	2.02	0.79
1:B:253:LYS:HB3	8:B:657:HOH:O	1.82	0.79
1:E:298:SER:HB3	1:E:301:GLU:HB2	1.64	0.79
1:D:16[A]:HIS:CD2	2:Y:501:A:C2	2.71	0.78
1:E:319[B]:GLU:OE1	1:E:324:LEU:HD12	1.83	0.78
1:B:63:LYS:HE2	1:B:64:TYR:CZ	2.18	0.78
1:B:16[B]:HIS:CE1	3:R:510:G46:S2P	2.76	0.77
1:E:91[B]:HIS:NE2	2:Z:502:C:O3'	2.18	0.77
1:B:310:LEU:HD22	8:B:675:HOH:O	1.86	0.75
1:D:253:LYS:HD2	1:D:253:LYS:O	1.86	0.75
1:E:16[A]:HIS:NE2	2:Z:503:A:OP1	2.21	0.73
1:D:16[A]:HIS:NE2	3:T:510:G46:S2P	2.59	0.73
1:D:41:ILE:HG21	1:D:178:LEU:HD11	1.69	0.72
1:D:308:LYS:NZ	1:D:308:LYS:HB3	2.04	0.72
1:A:253:LYS:HD2	1:A:253:LYS:O	1.90	0.72
1:B:14:SER:OG	1:B:16[B]:HIS:CD2	2.44	0.71
1:B:141:PRO:HD2	7:B:403:PG4:C5	2.17	0.71
1:B:301:GLU:OE1	1:B:305:LYS:HE3	1.90	0.71
1:A:16:HIS:HE1	1:A:91:HIS:HD2	1.40	0.70
1:B:41:ILE:HG21	1:B:178:LEU:HD11	1.74	0.69
1:D:91:HIS:HE1	2:Y:501:A:C2'	2.05	0.69
1:E:234:GLU:OE2	1:E:236:HIS:ND1	2.26	0.69
1:D:230:HIS:HA	8:D:800:HOH:O	1.93	0.69
1:B:91:HIS:NE2	3:R:510:G46:O3P	2.25	0.68
1:D:308:LYS:NZ	1:D:308:LYS:CB	2.55	0.68
1:B:319:GLU:OE1	1:B:324:LEU:HG	1.94	0.68
1:C:138:GLU:HG2	1:C:159:ASN:HB2	1.74	0.68
1:C:21[B]:GLU:OE1	1:C:24:ARG:NH1	2.27	0.67
1:B:16[A]:HIS:NE2	1:B:18:LYS:HD2	2.08	0.67
1:A:262:PRO:HG2	8:A:808:HOH:O	1.94	0.67
1:A:16:HIS:NE2	3:Q:510:G46:S2P	2.67	0.66
1:A:91:HIS:NE2	2:V:501:A:H1'	2.11	0.66
1:D:146:PRO:HG2	5:D:402:SO4:O4	1.96	0.66
1:B:325:LYS:HG2	8:B:621:HOH:O	1.95	0.66
2:Y:501:A:OP1	2:Y:501:A:C3'	2.39	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:HD21	1:C:231:MET:HE1	1.76	0.65
1:E:264:LYS:HD2	1:E:265:GLN:HE21	1.60	0.65
1:C:151:VAL:HG13	1:C:152:VAL:HG13	1.78	0.65
1:C:72:LEU:HD12	1:C:77:LYS:HD2	1.78	0.64
1:C:313:LYS:HD2	1:C:317:LEU:CD2	2.28	0.64
1:A:194:GLN:O	1:A:198:PHE:HD1	1.81	0.64
1:D:41:ILE:HG23	1:D:178:LEU:HD21	1.80	0.64
1:A:71:HIS:CE1	1:A:72:LEU:CD1	2.81	0.64
1:A:232:HIS:NE2	3:Q:510:G46:S2P	2.70	0.64
1:D:16[A]:HIS:CE1	3:T:510:G46:HS	2.11	0.63
1:D:231:MET:O	1:D:232:HIS:HB2	1.97	0.63
1:E:46:MET:HG3	1:E:86:PHE:CD2	2.34	0.63
1:B:140:LYS:HG3	7:B:403:PG4:C5	2.28	0.63
1:B:140:LYS:HG3	7:B:403:PG4:H51	1.81	0.63
1:A:27:SER:OG	1:A:31:LYS:NZ	2.28	0.63
1:B:200:PRO:O	1:B:203:LYS:HB2	1.99	0.63
1:E:273:LYS:HG2	1:E:315:ILE:HD12	1.82	0.62
1:D:8:HIS:ND1	1:D:260:ASP:OD1	2.29	0.62
1:E:16[A]:HIS:CE1	2:Z:503:A:OP1	2.52	0.62
1:C:71:HIS:CE1	1:C:72:LEU:HD13	2.35	0.62
1:C:313:LYS:HD2	1:C:317:LEU:HD22	1.80	0.62
1:D:308:LYS:HB3	1:D:308:LYS:HZ3	1.64	0.62
1:B:91:HIS:NE2	2:W:501:A:H1'	2.15	0.61
1:D:6:ILE:HG13	1:D:7:GLN:N	2.15	0.61
1:C:312:LYS:HD3	8:C:660:HOH:O	2.02	0.60
1:A:16:HIS:CE1	3:Q:510:G46:S2P	2.95	0.60
1:D:6:ILE:CD1	1:D:260:ASP:HB3	2.32	0.60
1:D:205:ASP:OD1	1:D:205:ASP:N	2.34	0.59
1:E:63:LYS:HE2	1:E:64:TYR:CZ	2.38	0.59
1:C:41:ILE:HG23	1:C:178:LEU:HD21	1.84	0.59
1:E:313:LYS:O	1:E:317:LEU:HD13	2.03	0.59
1:E:6:ILE:HD11	1:E:8:HIS:CE1	2.38	0.59
1:D:47:GLN:HE22	2:Y:501:A:H2	1.50	0.59
1:B:91:HIS:HE2	2:W:501:A:H1'	1.69	0.58
1:E:6:ILE:HD12	1:E:260:ASP:HB3	1.86	0.58
1:B:16[A]:HIS:CE1	1:B:18:LYS:HD2	2.38	0.58
1:C:112:TYR:CE2	1:C:114:GLY:HA2	2.39	0.57
1:B:154:LEU:HD21	7:B:403:PG4:H11	1.85	0.57
1:D:204:LYS:HB2	8:D:799:HOH:O	2.04	0.57
1:E:173:GLN:OE1	1:E:224:LYS:NZ	2.36	0.57
1:E:75:GLU:OE2	1:E:77:LYS:HE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:CG	1:A:145:PRO:HA	2.40	0.57
1:C:232:HIS:HE1	8:C:707:HOH:O	1.87	0.57
1:E:309:GLU:HG2	8:E:775:HOH:O	2.04	0.57
1:B:218:LEU:O	1:B:218:LEU:HD23	2.04	0.56
1:E:264:LYS:CD	1:E:265:GLN:HB3	2.35	0.56
1:C:313:LYS:O	1:C:317:LEU:CD2	2.52	0.56
1:E:59:LYS:O	1:E:59:LYS:HG3	2.05	0.56
1:E:173:GLN:OE1	1:E:224:LYS:CE	2.53	0.56
1:E:119:ILE:C	1:E:119:ILE:HD12	2.26	0.56
1:D:252:TYR:N	1:D:252:TYR:CD1	2.73	0.55
1:E:272:ASP:O	1:E:276:VAL:HG23	2.05	0.55
1:A:175:ASP:OD1	1:A:224:LYS:HE3	2.07	0.55
1:A:197:ARG:NE	8:A:824:HOH:O	2.35	0.55
1:B:218:LEU:HD23	1:B:218:LEU:C	2.27	0.55
1:A:232:HIS:CE1	3:Q:510:G46:S2P	3.00	0.55
1:C:182:TRP:CE2	1:C:231:MET:HG3	2.41	0.55
1:C:151:VAL:HG13	1:C:152:VAL:N	2.22	0.55
1:E:173:GLN:OE1	1:E:224:LYS:HE3	2.07	0.55
1:A:148:PRO:HG3	8:A:818:HOH:O	2.08	0.54
1:A:16:HIS:HE1	1:A:91:HIS:CD2	2.22	0.54
1:E:298:SER:CB	1:E:301:GLU:HB2	2.33	0.54
2:Y:501:A:H3'	2:Y:501:A:P	2.48	0.54
1:A:71:HIS:CE1	1:A:72:LEU:HD13	2.42	0.54
1:D:59:LYS:HD2	1:D:59:LYS:C	2.27	0.54
1:D:46:MET:HG3	1:D:86:PHE:CD2	2.43	0.53
1:E:49:LEU:HD12	1:E:93:SER:HB2	1.90	0.53
1:A:46:MET:HG3	1:A:86:PHE:CD1	2.43	0.53
1:E:71:HIS:CE1	1:E:72:LEU:HD13	2.44	0.53
1:E:298:SER:HB3	1:E:301:GLU:CB	2.35	0.53
1:B:16[A]:HIS:HE1	1:B:250:ILE:O	1.92	0.53
1:D:16[A]:HIS:HD2	2:Y:501:A:N1	2.05	0.53
1:E:16[B]:HIS:HE1	2:Z:502:C:O2	1.91	0.53
1:B:253:LYS:HD2	1:B:253:LYS:O	2.09	0.52
1:C:79:LYS:HE3	8:C:773:HOH:O	2.08	0.52
1:D:41:ILE:CG2	1:D:178:LEU:HD21	2.39	0.52
1:C:41:ILE:HG21	1:C:178:LEU:HD11	1.90	0.52
1:A:41:ILE:CG2	1:A:178:LEU:HD21	2.40	0.52
1:E:264:LYS:HD3	1:E:265:GLN:HB3	1.92	0.52
1:C:77:LYS:HE3	8:C:543:HOH:O	2.10	0.52
1:D:29:TYR:OH	1:D:35:LYS:HD3	2.08	0.52
1:B:154:LEU:HD21	7:B:403:PG4:C1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:CE1	3:Q:510:G46:HA	2.27	0.52
1:A:234:GLU:HB2	1:A:254:ASN:HB2	1.92	0.52
1:E:173:GLN:HE22	1:E:224:LYS:CE	2.08	0.52
1:B:91:HIS:HE2	2:W:501:A:C2'	2.23	0.51
1:E:5:GLN:HB2	8:E:742:HOH:O	2.09	0.51
1:E:27:SER:O	1:E:31:LYS:HG3	2.10	0.51
1:B:265:GLN:O	1:B:265:GLN:HG2	2.08	0.51
1:D:144:TYR:CG	1:D:145:PRO:HA	2.45	0.51
1:B:298:SER:HB3	1:B:301:GLU:HB3	1.91	0.51
1:A:91:HIS:NE2	3:Q:510:G46:O3P	2.32	0.51
1:A:91:HIS:HE2	2:V:501:A:H1'	1.73	0.51
1:D:119:ILE:HD12	1:D:119:ILE:C	2.31	0.51
1:B:16[B]:HIS:CE1	3:R:510:G46:HS	2.26	0.51
1:C:29:TYR:OH	1:C:35:LYS:HD3	2.10	0.50
1:E:232:HIS:CE1	2:Z:503:A:H3'	2.47	0.50
1:E:79:LYS:HE2	1:E:108:PHE:CD2	2.46	0.50
1:A:8:HIS:CE1	1:A:35:LYS:HD3	2.47	0.50
1:A:147:SER:HB3	1:A:150:ASP:OD2	2.11	0.50
1:A:159:ASN:ND2	8:A:603:HOH:O	2.30	0.50
1:B:21:GLU:HA	1:B:24:ARG:NH1	2.25	0.50
1:E:343:TYR:O	1:E:347:ILE:HG13	2.12	0.50
1:E:6:ILE:CD1	1:E:260:ASP:HB3	2.41	0.50
1:B:150:ASP:OD2	7:B:403:PG4:O1	2.25	0.50
1:C:151:VAL:HG13	1:C:152:VAL:CG1	2.42	0.50
1:D:16[B]:HIS:HE1	1:D:250:ILE:O	1.95	0.50
1:E:21:GLU:HA	1:E:24:ARG:NH1	2.27	0.50
1:D:253:LYS:NZ	8:D:744:HOH:O	2.45	0.49
1:A:96:VAL:HG13	1:A:333:PHE:CD2	2.47	0.49
1:C:86:PHE:CZ	1:C:112:TYR:HB2	2.47	0.49
1:C:151:VAL:CG1	1:C:152:VAL:HG13	2.41	0.49
1:E:6:ILE:HD11	1:E:8:HIS:HE1	1.76	0.49
1:E:47:GLN:NE2	1:E:91[A]:HIS:CD2	2.80	0.49
1:B:319:GLU:OE1	1:B:324:LEU:CG	2.59	0.49
1:C:265:GLN:CD	8:C:818:HOH:O	2.50	0.49
1:C:79:LYS:CE	8:C:773:HOH:O	2.60	0.49
1:D:16[B]:HIS:CD2	1:D:249:LYS:HE3	2.48	0.49
1:D:112:TYR:CE2	1:D:114:GLY:HA2	2.48	0.49
1:E:167:ASN:OD1	1:E:167:ASN:C	2.50	0.49
1:A:197:ARG:CD	8:A:824:HOH:O	2.60	0.49
1:E:30:GLU:HG2	1:E:35:LYS:O	2.12	0.49
1:D:319:GLU:HG3	8:D:705:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:GLN:HG2	8:E:502:HOH:O	2.12	0.48
1:B:141:PRO:HG2	7:B:403:PG4:H52	1.96	0.48
1:D:61:PRO:HG2	1:D:64:TYR:HD2	1.78	0.48
1:A:176:ILE:HG22	1:A:178:LEU:CD1	2.43	0.48
1:B:81:PRO:HG2	1:B:82:TYR:CD2	2.47	0.48
1:E:16[B]:HIS:CE1	2:Z:502:C:O2	2.66	0.48
1:E:144:TYR:HB3	1:E:289:LYS:O	2.13	0.48
1:D:308:LYS:CB	1:D:308:LYS:HZ2	2.24	0.48
1:E:268:ASP:HB2	1:E:325:LYS:CE	2.43	0.48
1:E:21:GLU:OE2	1:E:251:GLY:HA2	2.13	0.48
1:E:253:LYS:HA	1:E:253:LYS:HD2	1.77	0.48
1:A:313:LYS:HG3	1:A:317:LEU:HD22	1.96	0.48
1:B:249:LYS:O	1:B:255:ALA:HB2	2.13	0.48
1:E:91[B]:HIS:CD2	2:Z:502:C:C2'	2.94	0.48
1:A:232:HIS:CG	3:Q:510:G46:HA	2.30	0.48
1:C:81:PRO:HG2	1:C:82:TYR:CE1	2.49	0.48
1:A:27:SER:HG	1:A:31:LYS:HZ1	1.54	0.47
1:D:91:HIS:CE1	2:Y:501:A:C2'	2.89	0.47
1:E:194:GLN:CG	1:E:198:PHE:CE2	2.98	0.47
1:B:71:HIS:CE1	1:B:72:LEU:HD13	2.50	0.47
1:B:91:HIS:HE2	2:W:501:A:C1'	2.27	0.47
1:D:253:LYS:HD2	8:D:693:HOH:O	2.14	0.47
1:E:8:HIS:CD2	1:E:35:LYS:HB3	2.50	0.47
1:E:320:LYS:NZ	8:E:706:HOH:O	2.48	0.47
1:B:63:LYS:HB2	1:B:63:LYS:HE3	1.71	0.47
1:C:46:MET:HG3	1:C:86:PHE:CD1	2.50	0.47
1:A:11:ILE:HG21	1:A:227:ILE:HD13	1.97	0.46
1:A:140:LYS:HD2	8:A:521:HOH:O	2.14	0.46
1:A:145:PRO:CB	1:A:146:PRO:HD2	2.45	0.46
1:B:144:TYR:CG	1:B:145:PRO:HA	2.50	0.46
1:C:310:LEU:HD12	1:C:310:LEU:HA	1.68	0.46
1:C:144:TYR:CG	1:C:145:PRO:HA	2.51	0.46
1:D:59:LYS:HB2	1:D:151:VAL:HG22	1.96	0.46
1:E:319[B]:GLU:OE1	1:E:324:LEU:HB2	2.16	0.46
1:A:49:LEU:CD2	1:A:55:LEU:HD23	2.46	0.46
1:D:194:GLN:O	1:D:197:ARG:HB3	2.16	0.46
1:D:218:LEU:HD23	1:D:218:LEU:O	2.15	0.46
1:B:232:HIS:CE1	3:R:510:G46:H3'	2.50	0.46
2:Y:501:A:N6	8:Y:604:HOH:O	2.48	0.46
1:E:268:ASP:HB2	1:E:325:LYS:HE2	1.98	0.46
1:B:116:CYS:O	1:B:117:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LYS:HE2	8:B:766:HOH:O	2.16	0.45
1:E:132:ILE:CG2	1:E:180:HIS:HD2	2.29	0.45
1:C:166:SER:HB2	1:C:220:THR:HG21	1.98	0.45
1:D:91:HIS:CE1	3:T:510:G46:P	3.09	0.45
1:D:231:MET:O	1:D:232:HIS:CB	2.61	0.45
1:D:77:LYS:HE3	6:D:404:GOL:O3	2.17	0.45
1:E:18:LYS:HB2	1:E:250:ILE:HG21	1.97	0.45
1:B:134:LYS:HB3	1:B:136:PHE:CE1	2.51	0.45
1:B:281:MET:HG3	1:B:306:ARG:HG2	1.99	0.45
1:E:150:ASP:HB3	1:E:154:LEU:HG	1.99	0.45
1:A:310:LEU:HD12	1:A:310:LEU:HA	1.87	0.45
1:C:16:HIS:HE1	2:X:502:C:O2	2.00	0.45
1:D:137:ASP:OD2	1:D:156:HIS:ND1	2.41	0.45
1:E:234:GLU:OE2	1:E:236:HIS:CE1	2.70	0.45
1:A:60:VAL:HB	1:A:61:PRO:HD2	1.99	0.45
1:A:101:TYR:HB2	1:A:115:VAL:HG23	1.99	0.45
1:C:187:VAL:HG13	1:C:188:MET:N	2.32	0.45
1:C:204:LYS:HE3	1:C:204:LYS:HB2	1.24	0.45
1:E:195:LEU:HD21	1:E:202:PHE:HD2	1.81	0.45
1:B:283:TRP:CZ2	1:B:345:GLU:HB2	2.51	0.45
1:D:71:HIS:CE1	1:D:72:LEU:HD13	2.51	0.45
1:A:24:ARG:HG3	8:A:616:HOH:O	2.16	0.44
1:A:194:GLN:O	1:A:198:PHE:CD1	2.67	0.44
1:C:346:LYS:HE2	8:C:542:HOH:O	2.17	0.44
1:E:198:PHE:N	1:E:198:PHE:CD1	2.84	0.44
1:B:29:TYR:O	1:B:33:THR:HG23	2.17	0.44
1:D:6:ILE:HD11	1:D:260:ASP:HB3	1.98	0.44
1:D:16[A]:HIS:CD2	2:Y:501:A:N1	2.84	0.44
1:D:194:GLN:NE2	8:D:785:HOH:O	2.50	0.44
1:E:202:PHE:N	1:E:202:PHE:CD1	2.84	0.44
1:A:61:PRO:HG2	1:A:64:TYR:HD2	1.82	0.44
6:A:404:GOL:H2	8:A:791:HOH:O	2.17	0.44
1:B:193:LYS:HG2	8:B:503:HOH:O	2.17	0.44
1:B:179:SER:O	1:B:228:SER:HA	2.18	0.44
1:B:197:ARG:NH1	1:B:197:ARG:HG2	2.32	0.44
1:C:281:MET:HG3	1:C:306:ARG:HG2	2.00	0.44
1:D:308:LYS:HB3	1:D:308:LYS:HZ2	1.79	0.44
1:E:47:GLN:HE21	1:E:91[A]:HIS:CD2	2.36	0.44
1:E:270:GLU:OE2	1:E:325:LYS:HD3	2.17	0.44
1:C:295:LEU:HD23	1:C:295:LEU:HA	1.79	0.44
1:C:343:TYR:O	1:C:347:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ILE:HG21	1:E:178:LEU:HD11	2.00	0.44
1:E:321:TYR:CZ	1:E:346:LYS:HE3	2.53	0.44
1:C:151:VAL:CG1	1:C:152:VAL:N	2.80	0.43
1:D:173:GLN:NE2	8:D:683:HOH:O	2.47	0.43
1:D:267:THR:CG2	8:D:687:HOH:O	2.65	0.43
1:B:310:LEU:CD2	8:B:675:HOH:O	2.57	0.43
1:B:202:PHE:CD1	1:B:202:PHE:N	2.86	0.43
1:B:143:THR:CG2	7:B:403:PG4:C4	2.86	0.43
1:A:283:TRP:CZ2	1:A:345:GLU:HB2	2.53	0.43
1:B:292:PHE:HB2	1:B:293:PRO:HA	2.01	0.43
1:A:119:ILE:HD12	1:A:119:ILE:C	2.39	0.43
1:B:283:TRP:N	1:B:284:PRO:CD	2.82	0.43
1:D:273:LYS:HG3	8:D:590:HOH:O	2.18	0.43
1:B:46:MET:HG3	1:B:86:PHE:CD1	2.53	0.43
1:C:119:ILE:HD12	1:C:119:ILE:C	2.39	0.43
2:X:501:A:C2	2:X:503:A:C5	3.07	0.43
1:A:194:GLN:HG3	1:A:197:ARG:NH2	2.34	0.43
1:D:86:PHE:CZ	1:D:112:TYR:HB2	2.54	0.43
1:A:300:SER:O	8:A:789:HOH:O	2.21	0.42
1:D:29:TYR:CD1	1:D:29:TYR:C	2.93	0.42
1:A:27:SER:OG	1:A:31:LYS:CE	2.67	0.42
1:E:133:TYR:CZ	1:E:212:PRO:HG2	2.54	0.42
1:D:33:THR:HB	8:D:731:HOH:O	2.19	0.42
1:D:182:TRP:CE2	1:D:231:MET:HG2	2.54	0.42
1:D:257:SER:C	1:D:258:TYR:CD1	2.93	0.42
1:E:321:TYR:OH	1:E:346:LYS:HE3	2.19	0.42
1:B:133:TYR:HD1	1:B:213:ILE:HD12	1.85	0.42
1:C:71:HIS:O	1:C:75:GLU:HG3	2.19	0.42
1:C:310:LEU:HB3	8:C:578:HOH:O	2.19	0.42
1:E:13:GLY:HA3	1:E:248:GLY:O	2.19	0.42
1:A:315:ILE:HG13	8:A:822:HOH:O	2.19	0.42
1:B:320:LYS:CE	8:B:664:HOH:O	2.67	0.42
1:D:21:GLU:HG2	1:D:250:ILE:CG2	2.49	0.42
1:E:298:SER:O	1:E:302:LEU:HG	2.20	0.42
1:B:295:LEU:HD12	8:B:668:HOH:O	2.20	0.42
1:C:238:GLU:OE1	1:C:243:HIS:ND1	2.53	0.42
2:Z:501:A:C2	2:Z:503:A:C5	3.07	0.42
1:D:234:GLU:O	1:D:235:TYR:HB2	2.19	0.42
1:E:86:PHE:CZ	1:E:112:TYR:HB2	2.55	0.42
6:A:404:GOL:C2	8:A:791:HOH:O	2.68	0.41
1:B:288:ASN:C	1:B:288:ASN:OD1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ASP:O	1:D:70:PHE:C	2.58	0.41
1:D:218:LEU:HD23	1:D:218:LEU:C	2.40	0.41
1:E:280:ILE:HG13	1:E:314:ILE:HG23	2.02	0.41
1:B:134:LYS:HA	1:B:134:LYS:HD3	1.75	0.41
1:A:86:PHE:CZ	1:A:112:TYR:HB2	2.56	0.41
1:C:81:PRO:HG2	1:C:82:TYR:CD1	2.54	0.41
1:E:320:LYS:CE	8:E:507:HOH:O	2.68	0.41
1:C:310:LEU:HD21	1:C:353:ILE:HG21	2.02	0.41
1:C:247:LEU:HD23	1:C:247:LEU:HA	1.84	0.41
1:D:151:VAL:HG13	1:D:152:VAL:HG13	2.01	0.41
1:E:91[B]:HIS:CE1	8:E:578:HOH:O	2.73	0.41
1:B:141:PRO:HG2	7:B:403:PG4:C5	2.51	0.41
1:B:306:ARG:HA	8:B:763:HOH:O	2.21	0.41
1:B:14:SER:HG	1:B:16[B]:HIS:CD2	2.35	0.41
1:E:321:TYR:CZ	1:E:346:LYS:CE	3.04	0.41
1:A:99:HIS:O	1:A:337:PHE:HB2	2.21	0.41
1:B:215:LYS:HB3	1:B:215:LYS:HE2	1.70	0.41
1:C:134:LYS:HD2	1:C:136:PHE:CZ	2.56	0.41
1:D:209:LEU:C	1:D:209:LEU:CD2	2.89	0.41
1:A:81:PRO:HG2	1:A:82:TYR:CE2	2.56	0.41
1:C:232:HIS:CD2	2:X:503:A:H3'	2.56	0.41
1:D:271:TYR:HA	8:D:607:HOH:O	2.20	0.41
1:E:118:CYS:HA	1:E:126:ILE:O	2.19	0.41
1:A:21[B]:GLU:HA	1:A:21[B]:GLU:OE1	2.21	0.41
1:A:224:LYS:HA	8:A:525:HOH:O	2.20	0.41
1:B:112:TYR:CE2	1:B:114:GLY:HA2	2.56	0.41
1:C:253:LYS:HG3	1:C:253:LYS:O	2.21	0.41
1:C:118:CYS:HA	1:C:126:ILE:O	2.21	0.40
1:A:70:PHE:CE2	1:A:74:TYR:HB2	2.56	0.40
1:A:145:PRO:HB2	1:A:146:PRO:HD2	2.04	0.40
1:D:25:GLN:HG2	1:D:256:ILE:HD12	2.02	0.40
1:E:317:LEU:N	1:E:317:LEU:CD1	2.84	0.40
1:A:231:MET:O	1:A:232:HIS:HB2	2.21	0.40
1:B:61:PRO:HG2	1:B:64:TYR:HD2	1.87	0.40
1:C:134:LYS:HD2	1:C:136:PHE:CE1	2.57	0.40
1:B:16[A]:HIS:CE1	1:B:250:ILE:O	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/356 (98%)	342 (98%)	7 (2%)	1 (0%)	41	30
1	B	350/356 (98%)	342 (98%)	7 (2%)	1 (0%)	41	30
1	C	349/356 (98%)	341 (98%)	8 (2%)	0	100	100
1	D	349/356 (98%)	337 (97%)	11 (3%)	1 (0%)	41	30
1	E	349/356 (98%)	338 (97%)	11 (3%)	0	100	100
All	All	1747/1780 (98%)	1700 (97%)	44 (2%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
1	D	232	HIS
1	B	352	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/320 (99%)	310 (98%)	8 (2%)	47	38
1	B	319/320 (100%)	306 (96%)	13 (4%)	30	18
1	C	318/320 (99%)	302 (95%)	16 (5%)	24	11
1	D	318/320 (99%)	301 (95%)	17 (5%)	22	10
1	E	318/320 (99%)	304 (96%)	14 (4%)	28	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1591/1600 (99%)	1523 (96%)	68 (4%)	29 16

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	63	LYS
1	A	72	LEU
1	A	178	LEU
1	A	186	ILE
1	A	261	LEU
1	A	310	LEU
1	A	317	LEU
1	B	5	GLN
1	B	35	LYS
1	B	51	TYR
1	B	59	LYS
1	B	63	LYS
1	B	72	LEU
1	B	178	LEU
1	B	186	ILE
1	B	261	LEU
1	B	267	THR
1	B	301	GLU
1	B	310	LEU
1	B	317	LEU
1	C	16	HIS
1	C	27	SER
1	C	29	TYR
1	C	51	TYR
1	C	59	LYS
1	C	72	LEU
1	C	147	SER
1	C	178	LEU
1	C	199	GLN
1	C	204	LYS
1	C	231	MET
1	C	261	LEU
1	C	310	LEU
1	C	317	LEU
1	C	352	ASN
1	C	353	ILE

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Mol	Chain	Res	Type
1	D	6	ILE
1	D	18	LYS
1	D	29	TYR
1	D	31	LYS
1	D	51	TYR
1	D	66	GLN
1	D	72	LEU
1	D	173	GLN
1	D	178	LEU
1	D	205	ASP
1	D	209	LEU
1	D	231	MET
1	D	261	LEU
1	D	300	SER
1	D	308	LYS
1	D	310	LEU
1	D	352	ASN
1	E	6	ILE
1	E	36	GLU
1	E	51	TYR
1	E	72	LEU
1	E	147	SER
1	E	169	SER
1	E	178	LEU
1	E	204	LYS
1	E	253	LYS
1	E	261	LEU
1	E	265	GLN
1	E	300	SER
1	E	308	LYS
1	E	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	C	16	HIS
1	C	66	GLN
1	C	232	HIS
1	D	173	GLN
1	E	47	GLN
1	E	163	GLN

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Mol	Chain	Res	Type
1	E	265	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	V	0/5	-	-
2	W	1/5 (20%)	0	0
2	X	2/5 (40%)	1 (50%)	0
2	Y	0/5	-	-
2	Z	1/5 (20%)	0	0
3	Q	0/2	-	-
3	R	0/2	-	-
3	S	0/2	-	-
3	T	0/2	-	-
3	U	0/2	-	-
All	All	4/35 (11%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	502	C

There are no RNA pucker outliers to report.

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

Of 5 non-standard protein/DNA/RNA residues modelled in this entry, 1 is modelled with single atom - leaving 4 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	$\#\|Z\| > 2$
3	G46	Q	510	2,4	20,26,26	1.39	4 (20%)	22,40,40	1.29	2 (9%)
3	G46	R	510	2,4	11,13,26	1.25	1 (9%)	13,19,40	1.42	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	G46	T	510	2,4	2,4,26	2.39	1 (50%)	3,6,40	3.11	1 (33%)
3	G46	S	510	2	2,4,26	2.72	2 (100%)	3,6,40	2.70	1 (33%)

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	G46	Q	510	2,4	-	1/5/26/26	0/3/3/3
3	G46	R	510	2,4	-	1/5/19/26	0/1/1/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	510	G46	P-O1P	-3.25	1.48	1.56
3	S	510	G46	P-O1P	-3.24	1.48	1.56
3	Q	510	G46	P-O1P	-3.20	1.48	1.56
3	T	510	G46	P-O1P	-3.18	1.48	1.56
3	Q	510	G46	C6-N1	-2.26	1.34	1.37
3	Q	510	G46	C5-C4	2.18	1.48	1.43
3	Q	510	G46	P-O5'	2.11	1.61	1.57
3	S	510	G46	P-O5'	2.08	1.62	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	510	G46	O5'-P-O3P	-5.08	100.20	113.38
3	S	510	G46	O5'-P-O3P	-4.17	102.57	113.38
3	Q	510	G46	C3'-C2'-C1'	3.42	106.13	100.98
3	R	510	G46	O4'-C4'-C3'	3.02	107.38	104.70
3	Q	510	G46	C8-N7-C5	2.41	107.57	102.99
3	R	510	G46	O5'-C5'-C4'	-2.36	100.86	108.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	510	G46	O4'-C4'-C5'-O5'
3	R	510	G46	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	510	G46	7	0
3	R	510	G46	7	0
3	T	510	G46	7	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
5	SO4	D	402	-	4,4,4	0.22	0	6,6,6	0.72	0
5	SO4	B	402	-	4,4,4	0.12	0	6,6,6	0.40	0
6	GOL	A	403	-	5,5,5	0.31	0	5,5,5	0.48	0
6	GOL	C	403	-	5,5,5	0.34	0	5,5,5	0.69	0
5	SO4	A	402	-	4,4,4	0.82	0	6,6,6	1.38	1 (16%)
6	GOL	C	404	-	5,5,5	0.20	0	5,5,5	1.73	2 (40%)
6	GOL	A	404	-	5,5,5	0.53	0	5,5,5	0.39	0
6	GOL	D	404	-	5,5,5	0.33	0	5,5,5	0.75	0
5	SO4	C	402	-	4,4,4	0.18	0	6,6,6	0.51	0
5	SO4	E	402	-	4,4,4	0.16	0	6,6,6	0.23	0
7	PG4	B	403	-	12,12,12	0.64	0	11,11,11	0.39	0
6	GOL	D	403	-	5,5,5	0.32	0	5,5,5	0.66	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
6	GOL	A	403	-	-	1/4/4/4	-
6	GOL	C	403	-	-	3/4/4/4	-
6	GOL	C	404	-	-	2/4/4/4	-
6	GOL	A	404	-	-	0/4/4/4	-
6	GOL	D	404	-	-	4/4/4/4	-
7	PG4	B	403	-	-	4/10/10/10	-
6	GOL	D	403	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	402	SO4	O3-S-O1	3.08	125.40	109.31
6	C	404	GOL	C3-C2-C1	-2.82	100.76	111.70
6	C	404	GOL	O1-C1-C2	-2.46	98.42	110.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	403	GOL	C1-C2-C3-O3
6	D	404	GOL	O1-C1-C2-C3
6	D	404	GOL	C1-C2-C3-O3
7	B	403	PG4	O1-C1-C2-O2
7	B	403	PG4	O2-C3-C4-O3
7	B	403	PG4	O3-C5-C6-O4
6	A	403	GOL	C1-C2-C3-O3
6	C	404	GOL	O1-C1-C2-C3
7	B	403	PG4	O4-C7-C8-O5
6	C	403	GOL	O2-C2-C3-O3
6	C	404	GOL	O1-C1-C2-O2
6	D	404	GOL	O1-C1-C2-O2
6	D	404	GOL	O2-C2-C3-O3
6	C	403	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	402	SO4	1	0
6	C	404	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	404	GOL	2	0
6	D	404	GOL	1	0
7	B	403	PG4	14	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, 95^{th} 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	349/356 (98%)	0.21	17 (4%) 29 39	13, 22, 39, 55	0
1	B	349/356 (98%)	0.09	7 (2%) 65 73	13, 22, 39, 57	0
1	C	349/356 (98%)	0.25	11 (3%) 47 57	11, 21, 36, 57	0
1	D	349/356 (98%)	0.31	23 (6%) 18 26	11, 22, 45, 63	0
1	E	348/356 (97%)	0.35	22 (6%) 20 28	12, 25, 44, 58	0
2	V	3/5 (60%)	2.00	1 (33%) 0 0	39, 39, 40, 44	3 (100%)
2	W	3/5 (60%)	2.08	1 (33%) 0 0	37, 37, 42, 43	3 (100%)
2	X	3/5 (60%)	0.64	0 100 100	30, 30, 32, 45	2 (66%)
2	Y	2/5 (40%)	2.60	2 (100%) 0 0	47, 47, 47, 59	2 (100%)
2	Z	3/5 (60%)	1.66	1 (33%) 0 0	35, 35, 40, 49	3 (100%)
3	Q	0/2	-	-	-	-
3	R	0/2	-	-	-	-
3	S	0/2	-	-	-	-
3	T	0/2	-	-	-	-
3	U	0/2	-	-	-	-
All	All	1758/1815 (96%)	0.25	85 (4%) 30 40	11, 22, 42, 63	13 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	198	PHE	7.5
1	E	198	PHE	7.5
1	A	198	PHE	5.5
1	D	202	PHE	4.8
1	E	264	LYS	4.6
1	C	198	PHE	4.3
1	E	352	ASN	4.1
1	D	196	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
2	W	502	C	4.0
1	C	264	LYS	4.0
1	B	136	PHE	3.9
1	E	204	LYS	3.8
1	D	252	TYR	3.8
1	D	205	ASP	3.8
1	D	31	LYS	3.8
1	D	204	LYS	3.7
1	E	5	GLN	3.6
1	E	6	ILE	3.6
1	D	192	TYR	3.6
1	E	265	GLN	3.5
1	A	6	ILE	3.5
1	D	199	GLN	3.5
1	D	197	ARG	3.5
1	C	352	ASN	3.5
1	B	31	LYS	3.4
1	D	136	PHE	3.4
1	A	265	GLN	3.4
1	D	253	LYS	3.4
1	E	203	LYS	3.3
1	A	5	GLN	3.3
1	E	199	GLN	3.3
2	V	502	C	3.3
1	D	203	LYS	3.3
1	D	264	LYS	3.3
1	A	353	ILE	3.3
1	E	253	LYS	3.2
1	A	352	ASN	3.2
1	A	193	LYS	3.2
1	E	252	TYR	3.1
2	Z	501	A	3.1
1	E	33	THR	3.1
1	B	253	LYS	3.1
1	C	6	ILE	3.0
1	D	309	GLU	3.0
1	A	201	GLY	2.9
1	E	32	SER	2.9
1	E	202	PHE	2.9
2	Y	500	A	2.9
1	C	200	PRO	2.9
1	E	31	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	264	LYS	2.8
1	A	204	LYS	2.7
1	A	252	TYR	2.7
1	E	267	THR	2.7
1	E	206	GLY	2.6
1	D	352	ASN	2.5
1	C	31	LYS	2.5
1	D	193	LYS	2.5
1	A	263	LEU	2.5
1	B	265	GLN	2.4
1	A	194	GLN	2.4
1	E	29	TYR	2.4
1	C	115	VAL	2.4
2	Y	501	A	2.3
1	E	309	GLU	2.3
1	D	200	PRO	2.3
1	D	24	ARG	2.3
1	D	195	LEU	2.3
1	C	199	GLN	2.2
1	E	310	LEU	2.2
1	A	24	ARG	2.2
1	C	353	ILE	2.2
1	C	197	ARG	2.2
1	C	265	GLN	2.2
1	D	5	GLN	2.2
1	A	200	PRO	2.1
1	D	265	GLN	2.1
1	B	264	LYS	2.1
1	E	27	SER	2.1
1	A	33	THR	2.1
1	B	203	LYS	2.1
1	A	192	TYR	2.0
1	B	204	LYS	2.0
1	D	201	GLY	2.0
1	E	205	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, 95^{th} 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
3	G46	U	501	1/24	0.27	0.44	48,48,48,48	1
3	G46	S	510	5/24	0.60	0.25	47,50,58,62	5
3	G46	R	510	13/24	0.82	0.21	19,38,45,46	13
3	G46	Q	510	24/24	0.84	0.19	26,45,47,49	24
3	G46	T	510	5/24	0.91	0.13	24,44,46,52	5

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
6	GOL	A	404	6/6	0.75	0.25	30,34,43,44	0
6	GOL	D	404	6/6	0.83	0.24	23,32,38,38	0
7	PG4	B	403	13/13	0.84	0.40	24,34,47,50	0
6	GOL	A	403	6/6	0.86	0.17	26,35,37,44	0
6	GOL	C	404	6/6	0.86	0.29	31,36,40,42	0
6	GOL	C	403	6/6	0.87	0.20	32,35,44,45	0
6	GOL	D	403	6/6	0.87	0.19	28,32,44,47	0
5	SO4	B	402	5/5	0.97	0.10	34,35,39,49	0
5	SO4	C	402	5/5	0.97	0.12	33,33,37,43	0
5	SO4	A	402	5/5	0.97	0.10	31,35,37,38	0
5	SO4	E	402	5/5	0.98	0.10	28,29,35,46	0
5	SO4	D	402	5/5	0.98	0.12	28,28,37,47	0
4	NI	A	401	1/1	0.99	0.04	30,30,30,30	0
4	NI	B	401	1/1	0.99	0.05	23,23,23,23	0
4	NI	D	401	1/1	0.99	0.06	26,26,26,26	0
4	NI	E	401	1/1	0.99	0.09	21,21,21,21	0
4	NI	C	401	1/1	1.00	0.06	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.