WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:45 am GMT

PDB ID	:	4XRN
Title	:	Pilz domain with c-di-gmp of a protein from Pseudomonas aeruginosa
Authors	:	Chi, K.K.; Yuan, Z.L.
Deposited on	:	2015-01-21
Resolution	:	2.00 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:
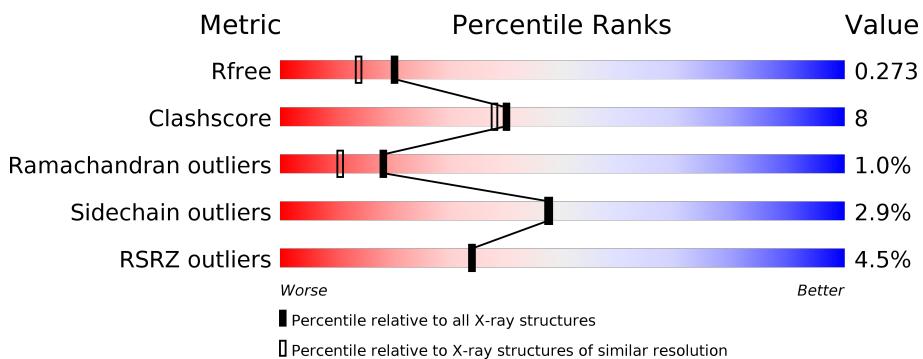
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
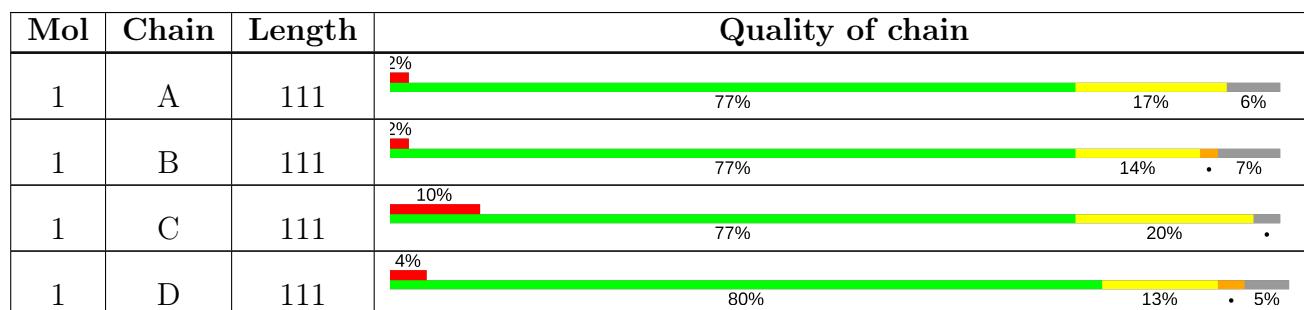
The reported resolution of this entry is 2.00 Å.

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	Percentile Ranks	Value
Rfree		0.273
Clashscore		8
Ramachandran outliers		1.0%
Sidechain outliers		2.9%
RSRZ outliers		4.5%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	111	2% / 77% / 17% / 6%
1	B	111	2% / 77% / 14% / • / 7%
1	C	111	10% / 77% / 20% / •
1	D	111	4% / 80% / 13% / • / 5%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4115 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.
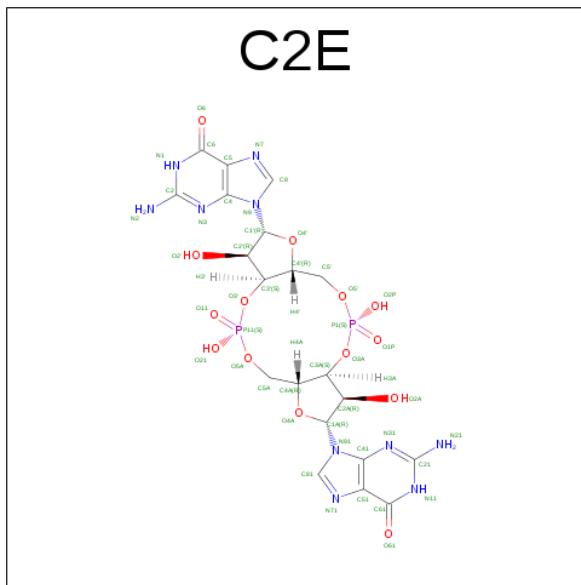
- Molecule 1 is a protein called Alginate biosynthesis protein Alg44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			809	513	149	146	1			
1	B	103	Total	C	N	O	S	0	0	0
			805	511	148	145	1			
1	C	108	Total	C	N	O	S	0	0	0
			838	533	153	151	1			
1	D	106	Total	C	N	O	S	0	0	0
			820	520	151	148	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9HY69
A	2	PRO	-	expression tag	UNP Q9HY69
A	3	GLY	-	expression tag	UNP Q9HY69
A	4	SER	-	expression tag	UNP Q9HY69
B	1	GLY	-	expression tag	UNP Q9HY69
B	2	PRO	-	expression tag	UNP Q9HY69
B	3	GLY	-	expression tag	UNP Q9HY69
B	4	SER	-	expression tag	UNP Q9HY69
C	1	GLY	-	expression tag	UNP Q9HY69
C	2	PRO	-	expression tag	UNP Q9HY69
C	3	GLY	-	expression tag	UNP Q9HY69
C	4	SER	-	expression tag	UNP Q9HY69
D	1	GLY	-	expression tag	UNP Q9HY69
D	2	PRO	-	expression tag	UNP Q9HY69
D	3	GLY	-	expression tag	UNP Q9HY69
D	4	SER	-	expression tag	UNP Q9HY69

- Molecule 2 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5 ,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclodode cine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	D	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	D	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	D	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total 5	Zn 5	0	0
3	A	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	C	1	Total 1	Zn 1	0	0
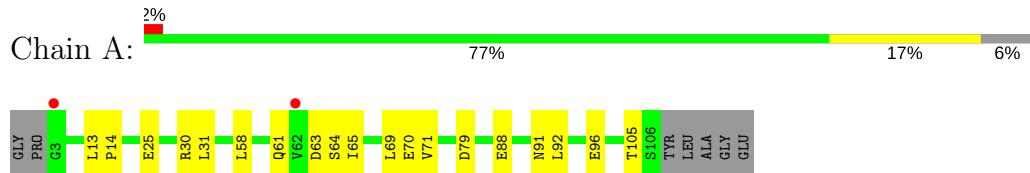
• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total 65	O 65	0	0
4	B	77	Total 77	O 77	0	0
4	C	73	Total 73	O 73	0	0
4	D	66	Total 66	O 66	0	0
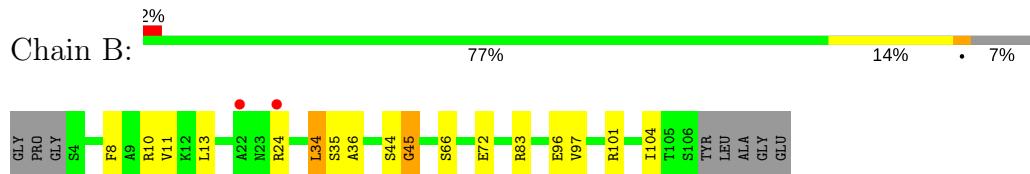
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.
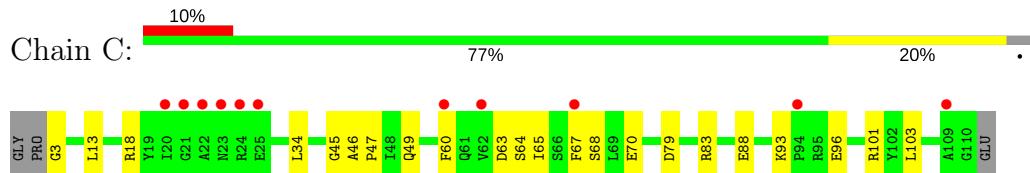
- Molecule 1: Alginate biosynthesis protein Alg44
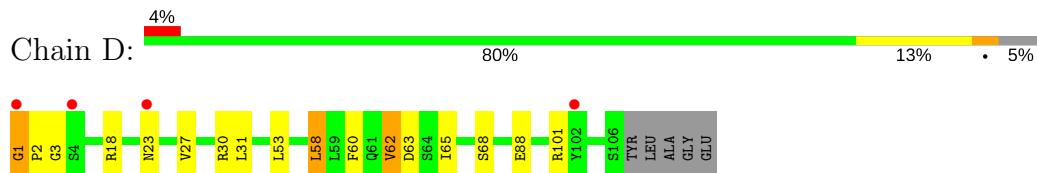
- Molecule 1: Alginate biosynthesis protein Alg44

- Molecule 1: Alginate biosynthesis protein Alg44

- Molecule 1: Alginate biosynthesis protein Alg44

4 Data and refinement statistics ⓘ

| Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	75.53Å 75.53Å 195.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.00 49.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.86-2.00) 98.8 (49.32-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.37 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1894)	Depositor
R, R_{free}	0.231 , 0.274 0.230 , 0.273	Depositor DCC
R_{free} test set	1983 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4115	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, C2E

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	0.41	0/823	0.54	0/1108
1	B	0.39	0/819	0.53	0/1103
1	C	0.38	0/853	0.56	0/1149
1	D	0.42	0/835	0.65	1/1125 (0.1%)
All	All	0.40	0/3330	0.57	1/4485 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	GLY	C-N-CD	-7.85	103.34	120.60

There are no chirality outliers.

There are no planarity outliers.

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	809	0	823	15	0
1	B	805	0	820	12	0
1	C	838	0	851	19	0
1	D	820	0	836	8	0
2	A	138	0	60	5	0
2	B	138	0	57	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	138	0	58	1	0
2	D	138	0	59	2	0
3	A	2	0	0	0	0
3	B	5	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	65	0	0	5	0
4	B	77	0	0	4	2
4	C	73	0	0	10	2
4	D	66	0	0	4	0
All	All	4115	0	3564	61	2

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 8.

All (61) 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)
2:A:202:C2E:H8	2:A:202:C2E:H5'2	1.38	1.03
1:C:88:GLU:OE2	4:C:301:HOH:O	1.89	0.90
1:D:88:GLU:OE2	4:D:301:HOH:O	1.89	0.89
1:C:83:ARG:NH2	4:C:305:HOH:O	2.14	0.79
1:A:30:ARG:NH2	4:A:302:HOH:O	2.15	0.78
1:C:63:ASP:OD2	4:C:302:HOH:O	2.04	0.75
1:A:65:ILE:HG23	1:C:67:PHE:HE1	1.54	0.73
1:C:63:ASP:OD1	4:C:303:HOH:O	2.09	0.70
1:B:96:GLU:OE2	4:B:301:HOH:O	2.09	0.69
2:A:202:C2E:H5'1	2:A:202:C2E:H3A	1.75	0.69
1:C:79:ASP:OD1	4:C:304:HOH:O	2.10	0.69
1:B:45:GLY:N	4:B:303:HOH:O	2.27	0.67
1:A:64:SER:OG	1:C:93:LYS:NZ	2.27	0.67
1:C:93:LYS:NZ	4:C:307:HOH:O	2.21	0.67
1:A:64:SER:HB3	1:C:70:GLU:HB3	1.75	0.67
2:A:202:C2E:C8	2:A:202:C2E:H5'2	2.22	0.67
1:A:88:GLU:OE2	4:A:301:HOH:O	2.13	0.66
1:B:72:GLU:OE2	4:B:302:HOH:O	2.12	0.66
1:D:63:ASP:OD2	4:D:302:HOH:O	2.13	0.66
2:B:201:C2E:H511	2:B:201:C2E:H3'	1.77	0.66
1:A:79:ASP:OD2	4:A:303:HOH:O	2.16	0.63
1:C:93:LYS:N	1:C:96:GLU:OE2	2.28	0.60
1:A:69:LEU:HG	1:A:71:VAL:HG13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:GLN:OE1	4:C:306:HOH:O	2.16	0.60
1:A:63:ASP:O	4:A:304:HOH:O	2.16	0.59
1:B:11:VAL:HG23	1:B:13:LEU:HD23	1.87	0.57
1:A:70:GLU:HB3	1:C:64:SER:HB3	1.86	0.57
1:D:62:VAL:HG13	1:D:65:ILE:HB	1.85	0.57
1:A:25:GLU:OE2	4:A:305:HOH:O	2.18	0.56
2:C:203:C2E:H2'	2:C:203:C2E:N3	2.19	0.55
1:C:13:LEU:HD11	1:C:34:LEU:HD23	1.91	0.52
2:A:201:C2E:O2P	2:A:202:C2E:N1	2.34	0.51
1:D:18:ARG:HA	1:D:27:VAL:O	2.11	0.51
1:A:31:LEU:HD11	1:A:58:LEU:HD11	1.93	0.49
1:A:96:GLU:HA	1:C:65:ILE:HD11	1.94	0.49
1:C:45:GLY:N	4:C:305:HOH:O	2.44	0.49
1:B:10:ARG:HG2	1:B:35:SER:HB3	1.94	0.48
2:D:203:C2E:H2'	2:D:203:C2E:N3	2.29	0.47
1:B:24:ARG:HD2	1:B:24:ARG:HA	1.71	0.47
1:B:8:PHE:CD1	1:B:36:ALA:HB3	2.51	0.46
1:C:46:ALA:HA	1:C:47:PRO:HD3	1.85	0.45
1:B:66:SER:HB3	1:D:68:SER:OG	2.17	0.45
1:B:34:LEU:HD13	1:B:104:ILE:HD11	1.98	0.45
1:A:63:ASP:HB3	1:A:64:SER:H	1.49	0.44
2:A:202:C2E:O5A	2:A:202:C2E:H81	2.19	0.43
2:B:202:C2E:O5'	2:B:202:C2E:H8	2.18	0.43
2:B:201:C2E:C81	2:B:201:C2E:H512	2.49	0.42
1:C:3:GLY:N	4:C:318:HOH:O	2.52	0.42
1:C:18:ARG:NH1	4:C:319:HOH:O	2.53	0.42
1:D:58:LEU:HB3	1:D:60:PHE:CE1	2.54	0.41
1:B:97:VAL:O	1:B:101:ARG:HG2	2.20	0.41
2:D:203:C2E:O6	4:D:303:HOH:O	2.22	0.41
1:B:44:SER:C	4:B:303:HOH:O	2.58	0.41
1:A:13:LEU:HB2	1:A:14:PRO:HD2	2.02	0.41
1:A:71:VAL:HG12	1:A:92:LEU:HD21	2.02	0.40
2:B:201:C2E:H512	2:B:201:C2E:H81	2.03	0.40
1:C:60:PHE:CE1	1:C:103:LEU:HD13	2.55	0.40
1:B:83:ARG:HA	1:B:83:ARG:HD2	1.89	0.40
2:B:201:C2E:H511	2:B:201:C2E:C3'	2.47	0.40
1:D:1:GLY:HA2	1:D:3:GLY:N	2.37	0.40
1:D:30:ARG:O	4:D:304:HOH:O	2.22	0.40

All (2) 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)
4:B:377:HOH:O	4:C:370:HOH:O[5_755]	2.03	0.17
4:B:364:HOH:O	4:C:357:HOH:O[4_574]	2.05	0.15

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	102/111 (92%)	97 (95%)	4 (4%)	1 (1%)	18	10
1	B	101/111 (91%)	98 (97%)	2 (2%)	1 (1%)	18	10
1	C	106/111 (96%)	104 (98%)	2 (2%)	0	100	100
1	D	104/111 (94%)	102 (98%)	0	2 (2%)	9	4
All	All	413/444 (93%)	401 (97%)	8 (2%)	4 (1%)	18	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	PRO
1	D	23	ASN
1	A	105	THR
1	B	45	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	84/88 (96%)	82 (98%)	2 (2%)	54	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	84/88 (96%)	83 (99%)	1 (1%)	75	80
1	C	86/88 (98%)	84 (98%)	2 (2%)	56	58
1	D	85/88 (97%)	80 (94%)	5 (6%)	23	17
All	All	339/352 (96%)	329 (97%)	10 (3%)	48	47

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	91	ASN
1	B	34	LEU
1	C	68	SER
1	C	101	ARG
1	D	31	LEU
1	D	53	LEU
1	D	58	LEU
1	D	62	VAL
1	D	101	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

Of 22 ligands modelled in this entry, 10 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	#$|Z| > 2$
2	C2E	A	201	-	44,52,52	5.47	32 (72%)	50,82,82	2.29	19 (38%)
2	C2E	A	202	-	44,52,52	5.42	32 (72%)	50,82,82	2.31	21 (42%)
2	C2E	A	203	3	44,52,52	5.51	33 (75%)	50,82,82	2.20	17 (34%)
2	C2E	B	201	-	44,52,52	5.51	32 (72%)	50,82,82	2.34	20 (40%)
2	C2E	B	202	3	44,52,52	5.43	34 (77%)	50,82,82	2.20	17 (34%)
2	C2E	B	203	3	44,52,52	5.45	32 (72%)	50,82,82	2.13	20 (40%)
2	C2E	C	201	-	44,52,52	5.39	32 (72%)	50,82,82	2.30	18 (36%)
2	C2E	C	202	-	44,52,52	5.28	32 (72%)	50,82,82	2.17	18 (36%)
2	C2E	C	203	3	44,52,52	5.45	33 (75%)	50,82,82	2.26	19 (38%)
2	C2E	D	201	-	44,52,52	5.39	31 (70%)	50,82,82	2.38	18 (36%)
2	C2E	D	202	-	44,52,52	5.43	33 (75%)	50,82,82	2.15	20 (40%)
2	C2E	D	203	3	44,52,52	5.49	33 (75%)	50,82,82	2.34	19 (38%)

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	C2E	A	201	-	-	0/22/62/62	0/6/7/7
2	C2E	A	202	-	-	0/22/62/62	0/6/7/7
2	C2E	A	203	3	-	0/22/62/62	0/6/7/7
2	C2E	B	201	-	-	0/22/62/62	0/6/7/7
2	C2E	B	202	3	-	0/22/62/62	0/6/7/7
2	C2E	B	203	3	-	0/22/62/62	0/6/7/7
2	C2E	C	201	-	-	0/22/62/62	0/6/7/7
2	C2E	C	202	-	-	0/22/62/62	0/6/7/7
2	C2E	C	203	3	-	0/22/62/62	0/6/7/7
2	C2E	D	201	-	-	0/22/62/62	0/6/7/7
2	C2E	D	202	-	-	0/22/62/62	0/6/7/7
2	C2E	D	203	3	-	0/22/62/62	0/6/7/7

All (389) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	203	C2E	C2'-C1'	-17.38	1.26	1.53
2	B	203	C2E	C2'-C1'	-17.23	1.26	1.53
2	B	202	C2E	C2'-C1'	-17.02	1.26	1.53
2	B	201	C2E	C2'-C1'	-16.79	1.27	1.53
2	A	201	C2E	C2'-C1'	-16.79	1.27	1.53
2	C	201	C2E	C2'-C1'	-16.64	1.27	1.53
2	D	202	C2E	C2'-C1'	-16.63	1.27	1.53
2	A	202	C2E	C2'-C1'	-16.63	1.27	1.53
2	D	203	C2E	C2'-C1'	-16.46	1.27	1.53
2	D	201	C2E	C2'-C1'	-16.10	1.28	1.53
2	C	203	C2E	C2'-C1'	-16.08	1.28	1.53
2	C	202	C2E	C2'-C1'	-15.88	1.28	1.53
2	A	201	C2E	C2A-C3A	-12.56	1.25	1.53
2	A	203	C2E	C2A-C3A	-12.50	1.25	1.53
2	B	202	C2E	C2A-C3A	-12.50	1.25	1.53
2	D	202	C2E	C2A-C3A	-12.49	1.25	1.53
2	D	203	C2E	C2A-C3A	-12.48	1.25	1.53
2	A	202	C2E	C2A-C3A	-12.47	1.25	1.53
2	C	203	C2E	C2A-C3A	-12.46	1.25	1.53
2	C	201	C2E	C2A-C3A	-12.42	1.25	1.53
2	B	201	C2E	C2A-C3A	-12.38	1.25	1.53
2	B	203	C2E	C2A-C3A	-12.24	1.25	1.53
2	D	201	C2E	C2A-C3A	-12.16	1.25	1.53
2	C	202	C2E	C2A-C3A	-11.90	1.26	1.53
2	A	201	C2E	C3'-C4'	-11.17	1.21	1.52
2	B	201	C2E	C3'-C4'	-11.12	1.22	1.52
2	A	203	C2E	C3'-C4'	-11.10	1.22	1.52
2	A	202	C2E	C3'-C4'	-10.91	1.22	1.52
2	D	203	C2E	C3'-C4'	-10.89	1.22	1.52
2	B	203	C2E	C3'-C4'	-10.87	1.22	1.52
2	B	202	C2E	C3'-C4'	-10.83	1.22	1.52
2	D	202	C2E	C3'-C4'	-10.83	1.22	1.52
2	C	201	C2E	C3'-C4'	-10.83	1.22	1.52
2	C	203	C2E	C3'-C4'	-10.78	1.23	1.52
2	D	201	C2E	C3'-C4'	-10.57	1.23	1.52
2	C	202	C2E	C3'-C4'	-10.54	1.23	1.52
2	D	202	C2E	O4A-C1A	-7.70	1.30	1.41
2	A	203	C2E	O4A-C1A	-7.27	1.31	1.41
2	B	201	C2E	O4A-C1A	-7.18	1.31	1.41
2	D	201	C2E	O4A-C1A	-7.16	1.31	1.41
2	C	203	C2E	O4A-C1A	-7.12	1.31	1.41
2	C	202	C2E	O4A-C1A	-6.94	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	C2E	O4A-C1A	-6.84	1.31	1.41
2	B	202	C2E	O4A-C1A	-6.71	1.32	1.41
2	C	201	C2E	O4A-C1A	-6.47	1.32	1.41
2	B	203	C2E	O4A-C1A	-6.46	1.32	1.41
2	D	203	C2E	O4A-C1A	-6.38	1.32	1.41
2	A	202	C2E	O4A-C1A	-6.31	1.32	1.41
2	B	201	C2E	C5A-C4A	-5.07	1.35	1.51
2	A	203	C2E	C5A-C4A	-4.92	1.36	1.51
2	A	202	C2E	C5A-C4A	-4.50	1.37	1.51
2	C	203	C2E	C5A-C4A	-4.46	1.37	1.51
2	D	201	C2E	C5A-C4A	-4.43	1.37	1.51
2	B	202	C2E	C5A-C4A	-4.43	1.37	1.51
2	D	203	C2E	C5A-C4A	-4.42	1.37	1.51
2	D	202	C2E	C5A-C4A	-4.37	1.37	1.51
2	A	201	C2E	C5A-C4A	-4.33	1.37	1.51
2	C	201	C2E	C5A-C4A	-4.22	1.38	1.51
2	B	203	C2E	C5A-C4A	-4.19	1.38	1.51
2	C	202	C2E	C5A-C4A	-4.05	1.38	1.51
2	D	201	C2E	O6-C6	-2.80	1.17	1.24
2	A	203	C2E	O6-C6	-2.78	1.17	1.24
2	B	203	C2E	O6-C6	-2.75	1.17	1.24
2	D	203	C2E	O6-C6	-2.62	1.18	1.24
2	B	202	C2E	O61-C61	-2.57	1.18	1.24
2	A	203	C2E	O61-C61	-2.55	1.18	1.24
2	C	203	C2E	O6-C6	-2.55	1.18	1.24
2	D	202	C2E	O6-C6	-2.46	1.18	1.24
2	A	201	C2E	O6-C6	-2.42	1.18	1.24
2	B	202	C2E	O6-C6	-2.40	1.18	1.24
2	C	201	C2E	O6-C6	-2.40	1.18	1.24
2	A	202	C2E	O6-C6	-2.40	1.18	1.24
2	A	202	C2E	O61-C61	-2.35	1.18	1.24
2	C	203	C2E	O61-C61	-2.35	1.18	1.24
2	A	203	C2E	C5-C4	-2.34	1.35	1.40
2	A	201	C2E	O61-C61	-2.34	1.18	1.24
2	B	201	C2E	O6-C6	-2.32	1.18	1.24
2	D	203	C2E	O61-C61	-2.31	1.18	1.24
2	C	202	C2E	O61-C61	-2.31	1.18	1.24
2	C	202	C2E	O6-C6	-2.31	1.18	1.24
2	C	201	C2E	O61-C61	-2.24	1.18	1.24
2	B	203	C2E	C5-C4	-2.19	1.35	1.40
2	D	201	C2E	O61-C61	-2.13	1.19	1.24
2	A	202	C2E	C5-C4	-2.10	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	202	C2E	C51-C41	-2.09	1.35	1.40
2	D	202	C2E	O61-C61	-2.09	1.19	1.24
2	D	201	C2E	C5-C4	-2.08	1.35	1.40
2	D	203	C2E	C5-C4	-2.07	1.35	1.40
2	B	201	C2E	C5-C4	-2.04	1.35	1.40
2	B	202	C2E	C51-C41	-2.03	1.35	1.40
2	B	202	C2E	C5-C4	-2.01	1.36	1.40
2	D	201	C2E	P1-O5'	2.01	1.67	1.59
2	C	201	C2E	C2-N3	2.03	1.45	1.35
2	C	202	C2E	P1-O3A	2.03	1.65	1.60
2	D	203	C2E	P1-O5'	2.03	1.67	1.59
2	C	203	C2E	P11-O5A	2.04	1.67	1.59
2	B	202	C2E	O2A-C2A	2.05	1.47	1.43
2	C	201	C2E	P11-O5A	2.05	1.67	1.59
2	C	201	C2E	O3A-C3A	2.07	1.52	1.44
2	D	202	C2E	P11-O5A	2.07	1.68	1.59
2	D	202	C2E	C21-N31	2.07	1.46	1.35
2	B	203	C2E	C21-N31	2.09	1.46	1.35
2	B	201	C2E	C21-N31	2.10	1.46	1.35
2	B	202	C2E	C21-N31	2.10	1.46	1.35
2	A	202	C2E	C21-N31	2.11	1.46	1.35
2	A	201	C2E	C21-N31	2.13	1.46	1.35
2	C	202	C2E	C21-N31	2.13	1.46	1.35
2	A	202	C2E	O2A-C2A	2.13	1.47	1.43
2	A	203	C2E	C2-N3	2.13	1.46	1.35
2	A	201	C2E	C2-N3	2.14	1.46	1.35
2	B	201	C2E	O2A-C2A	2.15	1.47	1.43
2	B	202	C2E	C2-N3	2.16	1.46	1.35
2	A	203	C2E	C21-N31	2.16	1.46	1.35
2	C	202	C2E	C2-N3	2.19	1.46	1.35
2	B	201	C2E	C2-N3	2.19	1.46	1.35
2	C	203	C2E	C21-N31	2.20	1.46	1.35
2	C	203	C2E	O3A-C3A	2.22	1.52	1.44
2	B	203	C2E	C2-N3	2.23	1.46	1.35
2	D	202	C2E	C2-N3	2.23	1.46	1.35
2	A	201	C2E	O3A-C3A	2.24	1.52	1.44
2	D	203	C2E	C2-N3	2.25	1.46	1.35
2	D	203	C2E	C21-N31	2.27	1.47	1.35
2	C	202	C2E	O4A-C4A	2.27	1.50	1.45
2	C	203	C2E	C2-N3	2.31	1.47	1.35
2	B	203	C2E	O2A-C2A	2.32	1.48	1.43
2	C	202	C2E	O3A-C3A	2.35	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	C2E	O3'-C3'	2.38	1.53	1.44
2	C	201	C2E	P1-O3A	2.39	1.66	1.60
2	B	203	C2E	O3'-C3'	2.39	1.53	1.44
2	D	202	C2E	O3A-C3A	2.39	1.53	1.44
2	B	203	C2E	P1-O5'	2.39	1.69	1.59
2	D	202	C2E	O2A-C2A	2.41	1.48	1.43
2	A	203	C2E	P1-O5'	2.41	1.69	1.59
2	D	201	C2E	O3'-C3'	2.42	1.53	1.44
2	A	203	C2E	O3'-C3'	2.44	1.53	1.44
2	B	202	C2E	O3A-C3A	2.46	1.53	1.44
2	A	201	C2E	O2A-C2A	2.47	1.48	1.43
2	C	203	C2E	O2A-C2A	2.47	1.48	1.43
2	C	201	C2E	P1-O5'	2.47	1.69	1.59
2	C	203	C2E	P1-O3A	2.49	1.67	1.60
2	D	203	C2E	O2A-C2A	2.49	1.48	1.43
2	D	202	C2E	O3'-C3'	2.53	1.53	1.44
2	B	201	C2E	O3A-C3A	2.54	1.53	1.44
2	B	202	C2E	P1-O5'	2.54	1.70	1.59
2	A	202	C2E	O3A-C3A	2.55	1.53	1.44
2	D	203	C2E	O3A-C3A	2.55	1.53	1.44
2	A	203	C2E	O2A-C2A	2.56	1.48	1.43
2	D	201	C2E	O4A-C4A	2.56	1.50	1.45
2	B	201	C2E	C3A-C4A	2.57	1.60	1.52
2	C	201	C2E	O4A-C4A	2.58	1.50	1.45
2	B	203	C2E	O3A-C3A	2.60	1.54	1.44
2	D	201	C2E	O3A-C3A	2.61	1.54	1.44
2	A	203	C2E	O3A-C3A	2.65	1.54	1.44
2	C	203	C2E	O4A-C4A	2.65	1.51	1.45
2	B	201	C2E	O3'-C3'	2.67	1.54	1.44
2	B	201	C2E	P1-O3A	2.68	1.67	1.60
2	C	202	C2E	P1-O5'	2.69	1.70	1.59
2	C	203	C2E	O3'-C3'	2.69	1.54	1.44
2	D	201	C2E	O2A-C2A	2.71	1.49	1.43
2	A	201	C2E	O3'-C3'	2.72	1.54	1.44
2	D	203	C2E	C5'-C4'	2.72	1.60	1.51
2	D	202	C2E	P1-O5'	2.73	1.70	1.59
2	A	201	C2E	P1-O3A	2.73	1.67	1.60
2	C	203	C2E	P1-O5'	2.73	1.70	1.59
2	B	202	C2E	O3'-C3'	2.74	1.54	1.44
2	A	202	C2E	O4A-C4A	2.74	1.51	1.45
2	C	202	C2E	O3'-C3'	2.75	1.54	1.44
2	B	202	C2E	O4A-C4A	2.77	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	203	C2E	O4A-C4A	2.77	1.51	1.45
2	D	203	C2E	O3'-C3'	2.81	1.54	1.44
2	A	201	C2E	P1-O5'	2.82	1.71	1.59
2	A	202	C2E	C5'-C4'	2.85	1.60	1.51
2	D	202	C2E	P1-O3A	2.86	1.67	1.60
2	A	203	C2E	P1-O3A	2.86	1.67	1.60
2	A	201	C2E	O4A-C4A	2.89	1.51	1.45
2	B	201	C2E	P1-O5'	2.90	1.71	1.59
2	B	201	C2E	O4A-C4A	2.90	1.51	1.45
2	C	202	C2E	O2A-C2A	2.94	1.49	1.43
2	D	203	C2E	P1-O3A	2.96	1.68	1.60
2	D	202	C2E	C5'-C4'	2.97	1.61	1.51
2	D	202	C2E	O4A-C4A	3.00	1.51	1.45
2	C	203	C2E	C3A-C4A	3.00	1.61	1.52
2	A	202	C2E	O3'-C3'	3.01	1.55	1.44
2	C	203	C2E	C5'-C4'	3.01	1.61	1.51
2	C	201	C2E	O2A-C2A	3.04	1.49	1.43
2	B	203	C2E	O4A-C4A	3.04	1.51	1.45
2	A	201	C2E	C3A-C4A	3.09	1.61	1.52
2	A	203	C2E	C5'-C4'	3.09	1.61	1.51
2	D	202	C2E	C3A-C4A	3.09	1.61	1.52
2	B	203	C2E	C3A-C4A	3.13	1.61	1.52
2	D	201	C2E	P1-O3A	3.14	1.68	1.60
2	C	202	C2E	C3A-C4A	3.14	1.61	1.52
2	D	203	C2E	C3A-C4A	3.14	1.61	1.52
2	B	202	C2E	P1-O3A	3.16	1.68	1.60
2	A	201	C2E	C5'-C4'	3.24	1.61	1.51
2	C	201	C2E	C5'-C4'	3.30	1.62	1.51
2	D	203	C2E	O4A-C4A	3.30	1.52	1.45
2	B	203	C2E	C5'-C4'	3.31	1.62	1.51
2	B	202	C2E	C5'-C4'	3.32	1.62	1.51
2	B	203	C2E	P1-O3A	3.32	1.69	1.60
2	C	202	C2E	C5'-C4'	3.34	1.62	1.51
2	A	202	C2E	P1-O3A	3.35	1.69	1.60
2	D	201	C2E	C5'-C4'	3.36	1.62	1.51
2	A	203	C2E	C3A-C4A	3.44	1.62	1.52
2	D	201	C2E	C3A-C4A	3.48	1.62	1.52
2	B	202	C2E	C3A-C4A	3.48	1.62	1.52
2	B	201	C2E	C5'-C4'	3.48	1.62	1.51
2	A	202	C2E	C3A-C4A	3.53	1.62	1.52
2	C	201	C2E	C3A-C4A	3.69	1.63	1.52
2	D	203	C2E	C2-N1	4.12	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	C2E	C2-N1	4.14	1.42	1.35
2	C	202	C2E	C2-N1	4.23	1.43	1.35
2	D	202	C2E	C2-N1	4.24	1.43	1.35
2	A	203	C2E	C2-N1	4.26	1.43	1.35
2	C	201	C2E	C2-N1	4.36	1.43	1.35
2	B	203	C2E	C2-N1	4.41	1.43	1.35
2	D	202	C2E	C2-N2	4.47	1.43	1.34
2	C	203	C2E	C2-N1	4.48	1.43	1.35
2	D	201	C2E	C2-N1	4.50	1.43	1.35
2	B	201	C2E	C2-N1	4.55	1.43	1.35
2	A	201	C2E	C2-N1	4.55	1.43	1.35
2	C	203	C2E	P11-O3'	4.57	1.72	1.60
2	C	203	C2E	C2-N2	4.58	1.43	1.34
2	C	202	C2E	P11-O3'	4.64	1.72	1.60
2	B	203	C2E	C2-N2	4.68	1.43	1.34
2	B	203	C2E	P11-O3'	4.72	1.72	1.60
2	C	202	C2E	C2-N2	4.79	1.43	1.34
2	D	201	C2E	C2-N2	4.81	1.43	1.34
2	A	202	C2E	C2-N1	4.82	1.44	1.35
2	D	201	C2E	P11-O3'	4.84	1.72	1.60
2	B	202	C2E	C2-N2	4.89	1.44	1.34
2	B	202	C2E	C6-N1	4.90	1.41	1.33
2	D	203	C2E	C2-N2	4.93	1.44	1.34
2	A	201	C2E	C2-N2	4.99	1.44	1.34
2	C	203	C2E	C6-N1	5.04	1.42	1.33
2	A	201	C2E	P11-O3'	5.04	1.73	1.60
2	B	201	C2E	C2-N2	5.04	1.44	1.34
2	B	201	C2E	C6-N1	5.07	1.42	1.33
2	A	202	C2E	P11-O3'	5.11	1.73	1.60
2	A	203	C2E	C21-N11	5.13	1.44	1.35
2	D	202	C2E	P11-O3'	5.13	1.73	1.60
2	A	203	C2E	C2-N2	5.14	1.44	1.34
2	D	203	C2E	C21-N11	5.16	1.44	1.35
2	C	201	C2E	P11-O3'	5.16	1.73	1.60
2	C	201	C2E	C2-N2	5.17	1.44	1.34
2	A	202	C2E	C2-N2	5.23	1.44	1.34
2	C	202	C2E	O4'-C4'	5.23	1.56	1.45
2	D	202	C2E	O4'-C4'	5.25	1.56	1.45
2	D	201	C2E	O4'-C4'	5.25	1.56	1.45
2	B	202	C2E	P11-O3'	5.26	1.74	1.60
2	B	203	C2E	C6-N1	5.27	1.42	1.33
2	D	202	C2E	C21-N11	5.27	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	202	C2E	C6-N1	5.28	1.42	1.33
2	B	201	C2E	O4'-C4'	5.29	1.57	1.45
2	D	201	C2E	C21-N11	5.32	1.45	1.35
2	A	201	C2E	C21-N11	5.33	1.45	1.35
2	A	203	C2E	O4'-C4'	5.33	1.57	1.45
2	C	201	C2E	C6-N1	5.36	1.42	1.33
2	C	201	C2E	O4'-C4'	5.37	1.57	1.45
2	C	201	C2E	C21-N11	5.39	1.45	1.35
2	A	203	C2E	P11-O3'	5.40	1.74	1.60
2	B	203	C2E	C21-N11	5.40	1.45	1.35
2	A	201	C2E	O4'-C4'	5.43	1.57	1.45
2	B	202	C2E	C21-N11	5.44	1.45	1.35
2	A	203	C2E	C6-N1	5.44	1.42	1.33
2	B	201	C2E	P11-O3'	5.47	1.74	1.60
2	A	202	C2E	C21-N11	5.47	1.45	1.35
2	A	201	C2E	C6-N1	5.48	1.43	1.33
2	B	203	C2E	O4'-C4'	5.49	1.57	1.45
2	B	202	C2E	O4'-C4'	5.50	1.57	1.45
2	D	203	C2E	C6-N1	5.51	1.43	1.33
2	D	203	C2E	P11-O3'	5.51	1.74	1.60
2	B	201	C2E	C21-N11	5.53	1.45	1.35
2	C	201	C2E	C2'-C3'	5.59	1.65	1.53
2	D	201	C2E	C6-N1	5.61	1.43	1.33
2	C	202	C2E	C21-N11	5.61	1.45	1.35
2	A	202	C2E	C6-N1	5.68	1.43	1.33
2	C	203	C2E	C21-N11	5.71	1.45	1.35
2	C	203	C2E	C2'-C3'	5.77	1.65	1.53
2	D	203	C2E	C61-N11	5.78	1.43	1.33
2	D	203	C2E	O4'-C4'	5.79	1.58	1.45
2	B	202	C2E	C61-N11	5.83	1.43	1.33
2	B	203	C2E	C61-N11	5.84	1.43	1.33
2	D	202	C2E	C2'-C3'	5.89	1.66	1.53
2	A	202	C2E	C6-C5	5.89	1.52	1.41
2	C	203	C2E	O4'-C4'	5.91	1.58	1.45
2	A	202	C2E	O4'-C4'	5.91	1.58	1.45
2	A	203	C2E	C21-N21	5.91	1.46	1.34
2	A	201	C2E	C2'-C3'	5.91	1.66	1.53
2	A	202	C2E	C61-N11	5.94	1.43	1.33
2	A	201	C2E	O4'-C1'	5.95	1.49	1.41
2	A	201	C2E	C61-N11	5.96	1.43	1.33
2	B	201	C2E	C21-N21	5.97	1.46	1.34
2	D	202	C2E	C61-N11	5.97	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	C2E	C61-N11	6.00	1.43	1.33
2	A	203	C2E	C6-C5	6.00	1.52	1.41
2	D	201	C2E	C2'-C3'	6.01	1.66	1.53
2	A	201	C2E	C6-C5	6.02	1.52	1.41
2	B	202	C2E	C2'-C3'	6.06	1.66	1.53
2	D	202	C2E	C21-N21	6.09	1.46	1.34
2	A	203	C2E	C61-N11	6.10	1.44	1.33
2	D	202	C2E	C6-N1	6.11	1.44	1.33
2	C	201	C2E	C21-N21	6.18	1.46	1.34
2	C	202	C2E	C21-N21	6.18	1.46	1.34
2	B	202	C2E	C21-N21	6.19	1.46	1.34
2	D	201	C2E	C6-C5	6.23	1.53	1.41
2	C	202	C2E	C2'-C3'	6.24	1.67	1.53
2	D	203	C2E	C21-N21	6.25	1.46	1.34
2	A	202	C2E	C21-N21	6.26	1.46	1.34
2	C	201	C2E	C6-C5	6.28	1.53	1.41
2	B	202	C2E	C61-C51	6.29	1.53	1.41
2	C	202	C2E	C6-C5	6.29	1.53	1.41
2	B	201	C2E	C2'-C3'	6.31	1.67	1.53
2	B	201	C2E	C6-C5	6.31	1.53	1.41
2	A	203	C2E	C2'-C3'	6.31	1.67	1.53
2	B	203	C2E	C21-N21	6.32	1.47	1.34
2	B	202	C2E	C6-C5	6.32	1.53	1.41
2	C	202	C2E	C61-N11	6.33	1.44	1.33
2	B	203	C2E	C2'-C3'	6.35	1.67	1.53
2	A	202	C2E	C61-C51	6.40	1.53	1.41
2	C	203	C2E	C61-N11	6.41	1.44	1.33
2	D	202	C2E	C6-C5	6.42	1.53	1.41
2	A	202	C2E	C2'-C3'	6.42	1.67	1.53
2	C	201	C2E	C61-N11	6.43	1.44	1.33
2	C	203	C2E	C21-N21	6.43	1.47	1.34
2	D	201	C2E	C21-N21	6.44	1.47	1.34
2	D	201	C2E	C61-N11	6.50	1.44	1.33
2	C	201	C2E	C61-C51	6.52	1.53	1.41
2	D	202	C2E	C61-C51	6.53	1.53	1.41
2	D	201	C2E	O4'-C1'	6.59	1.50	1.41
2	D	203	C2E	C2'-C3'	6.62	1.67	1.53
2	A	203	C2E	C61-C51	6.67	1.54	1.41
2	C	202	C2E	C4-N3	6.69	1.46	1.35
2	C	203	C2E	C6-C5	6.71	1.54	1.41
2	B	201	C2E	O4'-C1'	6.72	1.50	1.41
2	A	203	C2E	O4'-C1'	6.72	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	203	C2E	C61-C51	6.72	1.54	1.41
2	A	201	C2E	C21-N21	6.76	1.47	1.34
2	D	203	C2E	C61-C51	6.78	1.54	1.41
2	B	203	C2E	C6-C5	6.79	1.54	1.41
2	D	203	C2E	C6-C5	6.80	1.54	1.41
2	A	202	C2E	C4-N3	6.80	1.46	1.35
2	C	202	C2E	C61-C51	6.84	1.54	1.41
2	A	203	C2E	C4-N3	6.84	1.46	1.35
2	B	203	C2E	C4-N3	6.87	1.46	1.35
2	C	202	C2E	O4'-C1'	6.90	1.50	1.41
2	D	202	C2E	O4'-C1'	6.98	1.50	1.41
2	B	202	C2E	C4-N3	6.99	1.47	1.35
2	C	201	C2E	C2A-C1A	7.00	1.64	1.53
2	D	202	C2E	C4-N3	7.02	1.47	1.35
2	C	201	C2E	O4'-C1'	7.04	1.51	1.41
2	D	201	C2E	C4-N3	7.05	1.47	1.35
2	C	203	C2E	C61-C51	7.06	1.54	1.41
2	C	203	C2E	O4'-C1'	7.08	1.51	1.41
2	A	201	C2E	C4-N3	7.09	1.47	1.35
2	A	202	C2E	O4'-C1'	7.10	1.51	1.41
2	B	202	C2E	O4'-C1'	7.10	1.51	1.41
2	D	201	C2E	C41-N31	7.17	1.47	1.35
2	A	201	C2E	C61-C51	7.23	1.55	1.41
2	C	201	C2E	C4-N3	7.30	1.47	1.35
2	D	201	C2E	C61-C51	7.33	1.55	1.41
2	C	203	C2E	C2A-C1A	7.36	1.65	1.53
2	D	203	C2E	C2A-C1A	7.43	1.65	1.53
2	B	201	C2E	C61-C51	7.48	1.55	1.41
2	B	203	C2E	O4'-C1'	7.49	1.51	1.41
2	C	202	C2E	C2A-C1A	7.60	1.65	1.53
2	A	202	C2E	C2A-C1A	7.64	1.65	1.53
2	B	201	C2E	C4-N3	7.67	1.48	1.35
2	C	203	C2E	C4-N3	7.74	1.48	1.35
2	B	202	C2E	C2A-C1A	7.76	1.66	1.53
2	B	203	C2E	C2A-C1A	7.80	1.66	1.53
2	A	202	C2E	C41-N31	7.80	1.48	1.35
2	B	203	C2E	C41-N31	7.82	1.48	1.35
2	D	203	C2E	C4-N3	7.82	1.48	1.35
2	D	202	C2E	C2A-C1A	7.87	1.66	1.53
2	C	202	C2E	C41-N31	7.93	1.48	1.35
2	A	203	C2E	C41-N31	7.96	1.48	1.35
2	B	201	C2E	C41-N31	8.00	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	C2E	C2A-C1A	8.03	1.66	1.53
2	D	203	C2E	O4'-C1'	8.07	1.52	1.41
2	A	203	C2E	C2A-C1A	8.22	1.66	1.53
2	D	202	C2E	C41-N31	8.30	1.49	1.35
2	B	202	C2E	C41-N31	8.31	1.49	1.35
2	B	201	C2E	C2A-C1A	8.31	1.66	1.53
2	D	203	C2E	C41-N31	8.38	1.49	1.35
2	C	201	C2E	C41-N31	8.49	1.49	1.35
2	D	201	C2E	C2A-C1A	8.72	1.67	1.53
2	A	201	C2E	C41-N31	8.78	1.50	1.35
2	C	203	C2E	C41-N31	8.84	1.50	1.35

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	201	C2E	C4'-O4'-C1'	-6.81	102.52	109.77
2	C	203	C2E	C4'-O4'-C1'	-5.84	103.55	109.77
2	D	201	C2E	N31-C21-N11	-5.57	119.33	127.46
2	D	203	C2E	N3-C2-N1	-5.54	119.37	127.46
2	A	201	C2E	N31-C21-N11	-5.39	119.58	127.46
2	B	202	C2E	C4'-O4'-C1'	-5.37	104.06	109.77
2	D	201	C2E	C1'-N9-C4	-5.34	117.41	126.64
2	B	201	C2E	N3-C2-N1	-5.19	119.87	127.46
2	C	203	C2E	N31-C21-N11	-5.13	119.97	127.46
2	C	203	C2E	N3-C2-N1	-5.12	119.99	127.46
2	A	202	C2E	C4'-O4'-C1'	-5.08	104.36	109.77
2	C	201	C2E	N31-C21-N11	-5.08	120.05	127.46
2	D	202	C2E	C4'-O4'-C1'	-5.07	104.38	109.77
2	D	201	C2E	N3-C2-N1	-5.05	120.09	127.46
2	A	201	C2E	N3-C2-N1	-5.02	120.12	127.46
2	A	203	C2E	N3-C2-N1	-5.02	120.13	127.46
2	C	202	C2E	C4'-O4'-C1'	-4.96	104.49	109.77
2	A	203	C2E	N31-C21-N11	-4.96	120.22	127.46
2	B	202	C2E	N31-C21-N11	-4.90	120.31	127.46
2	D	201	C2E	C4'-O4'-C1'	-4.88	104.58	109.77
2	D	203	C2E	N31-C21-N11	-4.87	120.35	127.46
2	A	203	C2E	C4'-O4'-C1'	-4.85	104.61	109.77
2	B	201	C2E	C4'-O4'-C1'	-4.83	104.63	109.77
2	D	202	C2E	N31-C21-N11	-4.75	120.52	127.46
2	B	203	C2E	N3-C2-N1	-4.74	120.54	127.46
2	B	203	C2E	N31-C21-N11	-4.69	120.61	127.46
2	A	202	C2E	N3-C2-N1	-4.69	120.61	127.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	C2E	N31-C21-N11	-4.69	120.61	127.46
2	C	202	C2E	C1'-N9-C4	-4.68	118.54	126.64
2	C	202	C2E	N31-C21-N11	-4.66	120.65	127.46
2	B	201	C2E	C1'-N9-C4	-4.56	118.76	126.64
2	B	202	C2E	N3-C2-N1	-4.55	120.82	127.46
2	A	202	C2E	N31-C21-N11	-4.55	120.82	127.46
2	D	203	C2E	C1'-N9-C4	-4.54	118.78	126.64
2	A	202	C2E	C1'-N9-C4	-4.52	118.82	126.64
2	C	202	C2E	N3-C2-N1	-4.52	120.86	127.46
2	C	201	C2E	N3-C2-N1	-4.45	120.97	127.46
2	A	201	C2E	C1'-N9-C4	-4.44	118.97	126.64
2	A	201	C2E	C4'-O4'-C1'	-4.40	105.09	109.77
2	B	202	C2E	C1'-N9-C4	-4.30	119.20	126.64
2	D	202	C2E	N3-C2-N1	-4.30	121.18	127.46
2	C	201	C2E	C1'-N9-C4	-4.21	119.36	126.64
2	B	203	C2E	C4'-O4'-C1'	-4.16	105.34	109.77
2	D	203	C2E	C4'-O4'-C1'	-4.04	105.47	109.77
2	A	203	C2E	C1'-N9-C4	-3.99	119.75	126.64
2	C	203	C2E	C1'-N9-C4	-3.96	119.79	126.64
2	A	202	C2E	C5'-C4'-C3'	-3.80	101.40	114.30
2	C	202	C2E	C5-C6-N1	-3.62	118.33	123.48
2	D	202	C2E	C1'-N9-C4	-3.58	120.44	126.64
2	B	203	C2E	C51-C61-N11	-3.53	118.46	123.48
2	B	201	C2E	C5-C6-N1	-3.49	118.52	123.48
2	C	201	C2E	C5-C6-N1	-3.47	118.54	123.48
2	B	201	C2E	C5A-C4A-C3A	-3.34	102.99	114.30
2	A	202	C2E	C5-C6-N1	-3.31	118.77	123.48
2	D	202	C2E	C51-C61-N11	-3.22	118.89	123.48
2	B	201	C2E	C51-C61-N11	-3.22	118.90	123.48
2	B	202	C2E	C5-C6-N1	-3.21	118.91	123.48
2	D	201	C2E	C41-C51-N71	-3.18	106.34	109.41
2	C	203	C2E	C5-C6-N1	-3.17	118.97	123.48
2	D	201	C2E	C5-C6-N1	-3.05	119.15	123.48
2	A	202	C2E	C51-C61-N11	-3.00	119.22	123.48
2	A	201	C2E	C4A-O4A-C1A	-2.92	106.66	109.77
2	B	203	C2E	C1'-N9-C4	-2.90	121.63	126.64
2	C	202	C2E	O2A-C2A-C1A	-2.86	102.67	111.61
2	A	201	C2E	C5-C6-N1	-2.82	119.46	123.48
2	B	201	C2E	C4A-O4A-C1A	-2.82	106.77	109.77
2	A	203	C2E	C5-C6-N1	-2.76	119.55	123.48
2	D	202	C2E	C5-C6-N1	-2.73	119.59	123.48
2	B	201	C2E	C41-C51-N71	-2.73	106.77	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	203	C2E	C51-C61-N11	-2.67	119.68	123.48
2	C	201	C2E	C51-C61-N11	-2.64	119.72	123.48
2	A	201	C2E	C51-C61-N11	-2.63	119.73	123.48
2	B	203	C2E	C5-C6-N1	-2.63	119.74	123.48
2	D	203	C2E	C51-C61-N11	-2.62	119.76	123.48
2	D	203	C2E	C4A-O4A-C1A	-2.60	107.00	109.77
2	D	202	C2E	C4A-O4A-C1A	-2.58	107.03	109.77
2	B	202	C2E	O2A-C2A-C1A	-2.56	103.61	111.61
2	C	201	C2E	O4A-C4A-C3A	-2.54	99.21	104.81
2	D	203	C2E	C6-C5-C4	-2.54	118.32	120.84
2	C	201	C2E	O3A-P1-O1P	-2.53	99.50	109.46
2	C	202	C2E	C51-C61-N11	-2.52	119.89	123.48
2	A	202	C2E	C41-C51-N71	-2.51	106.98	109.41
2	C	201	C2E	C4A-O4A-C1A	-2.37	107.24	109.77
2	D	201	C2E	C61-C51-C41	-2.37	118.49	120.84
2	A	201	C2E	O3A-P1-O1P	-2.35	100.22	109.46
2	D	202	C2E	O3'-P11-O11	-2.33	100.28	109.46
2	C	203	C2E	C51-C61-N11	-2.33	120.17	123.48
2	B	202	C2E	C51-C61-N11	-2.33	120.17	123.48
2	C	203	C2E	O2A-C2A-C1A	-2.32	104.34	111.61
2	D	203	C2E	C5-C6-N1	-2.31	120.20	123.48
2	D	201	C2E	C51-C61-N11	-2.28	120.24	123.48
2	B	203	C2E	O4A-C4A-C3A	-2.27	99.81	104.81
2	A	202	C2E	O2A-C2A-C1A	-2.27	104.51	111.61
2	C	202	C2E	O3A-P1-O1P	-2.25	100.61	109.46
2	B	203	C2E	C4-C5-N7	-2.24	107.24	109.41
2	D	202	C2E	C41-C51-N71	-2.24	107.24	109.41
2	D	202	C2E	O3A-P1-O1P	-2.22	100.73	109.46
2	C	201	C2E	O3'-P11-O11	-2.21	100.75	109.46
2	A	203	C2E	C4A-O4A-C1A	-2.21	107.41	109.77
2	D	201	C2E	C6-C5-C4	-2.21	118.65	120.84
2	A	201	C2E	C41-C51-N71	-2.21	107.28	109.41
2	B	202	C2E	O3A-P1-O1P	-2.20	100.80	109.46
2	D	202	C2E	C4-C5-N7	-2.19	107.30	109.41
2	B	203	C2E	O2A-C2A-C1A	-2.13	104.94	111.61
2	C	203	C2E	C4A-O4A-C1A	-2.13	107.50	109.77
2	C	203	C2E	C41-C51-N71	-2.11	107.38	109.41
2	C	203	C2E	O3'-P11-O11	-2.09	101.23	109.46
2	D	203	C2E	O2A-C2A-C1A	-2.07	105.14	111.61
2	D	202	C2E	O2A-C2A-C1A	-2.01	105.32	111.61
2	B	202	C2E	C2A-C3A-C4A	2.02	106.85	103.23
2	A	202	C2E	C2'-C3'-C4'	2.04	106.89	103.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	201	C2E	O2P-P1-O3A	2.05	114.72	106.49
2	C	202	C2E	O2A-C2A-C3A	2.06	117.03	111.18
2	B	203	C2E	C6-N1-C2	2.07	119.03	116.06
2	B	203	C2E	O2P-P1-O3A	2.11	114.97	106.49
2	D	202	C2E	C6-N1-C2	2.13	119.12	116.06
2	B	203	C2E	N2-C2-N1	2.16	120.69	117.24
2	D	202	C2E	O2P-P1-O3A	2.16	115.18	106.49
2	D	201	C2E	C61-N11-C21	2.18	119.19	116.06
2	A	202	C2E	O2P-P1-O5'	2.21	118.59	108.14
2	D	202	C2E	C3A-C2A-C1A	2.21	104.92	99.95
2	C	201	C2E	N21-C21-N11	2.22	120.79	117.24
2	C	202	C2E	C61-N11-C21	2.28	119.34	116.06
2	B	203	C2E	C3A-C2A-C1A	2.28	105.08	99.95
2	B	202	C2E	N2-C2-N1	2.30	120.91	117.24
2	B	201	C2E	O2P-P1-O3A	2.32	115.81	106.49
2	C	203	C2E	N2-C2-N1	2.33	120.97	117.24
2	A	201	C2E	N21-C21-N11	2.34	120.99	117.24
2	B	203	C2E	O21-P11-O3'	2.36	115.97	106.49
2	A	203	C2E	N2-C2-N1	2.36	121.02	117.24
2	A	201	C2E	N2-C2-N1	2.38	121.05	117.24
2	B	202	C2E	C3'-C2'-C1'	2.38	105.29	99.95
2	C	203	C2E	C61-N11-C21	2.39	119.49	116.06
2	D	203	C2E	O21-P11-O3'	2.40	116.14	106.49
2	A	202	C2E	C3'-C2'-C1'	2.42	105.39	99.95
2	B	203	C2E	N21-C21-N11	2.44	121.14	117.24
2	A	203	C2E	C61-N11-C21	2.44	119.57	116.06
2	C	203	C2E	C1A-N91-C41	2.45	130.87	126.64
2	D	203	C2E	C61-N11-C21	2.46	119.59	116.06
2	C	201	C2E	C61-N11-C21	2.46	119.60	116.06
2	A	202	C2E	N21-C21-N11	2.50	121.25	117.24
2	B	201	C2E	O21-P11-O5A	2.53	120.07	108.14
2	B	201	C2E	C2-N3-C4	2.54	118.12	115.16
2	A	203	C2E	C6-N1-C2	2.55	119.72	116.06
2	A	203	C2E	C3'-C2'-C1'	2.56	105.69	99.95
2	D	201	C2E	C3'-C2'-C1'	2.56	105.69	99.95
2	B	202	C2E	O21-P11-O3'	2.56	116.78	106.49
2	D	203	C2E	O2P-P1-O3A	2.57	116.80	106.49
2	C	202	C2E	C2-N3-C4	2.58	118.17	115.16
2	A	202	C2E	C6-N1-C2	2.59	119.78	116.06
2	A	201	C2E	O2P-P1-O3A	2.59	116.91	106.49
2	A	202	C2E	C2A-C3A-C4A	2.60	107.88	103.23
2	B	201	C2E	C3'-C2'-C1'	2.62	105.84	99.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	202	C2E	O21-P11-O3'	2.63	117.06	106.49
2	C	202	C2E	N21-C21-N11	2.65	121.47	117.24
2	C	203	C2E	O2P-P1-O3A	2.65	117.16	106.49
2	C	201	C2E	O2P-P1-O3A	2.66	117.17	106.49
2	B	201	C2E	C61-N11-C21	2.67	119.90	116.06
2	D	201	C2E	C1A-N91-C41	2.68	131.27	126.64
2	B	201	C2E	C3A-C2A-C1A	2.71	106.05	99.95
2	C	203	C2E	N21-C21-N11	2.72	121.59	117.24
2	A	201	C2E	C3'-C2'-C1'	2.73	106.09	99.95
2	C	201	C2E	C2-N3-C4	2.74	118.36	115.16
2	A	203	C2E	C3A-C2A-C1A	2.79	106.21	99.95
2	C	202	C2E	C3'-C2'-C1'	2.79	106.22	99.95
2	B	203	C2E	C61-N11-C21	2.81	120.09	116.06
2	A	201	C2E	C6-N1-C2	2.81	120.10	116.06
2	C	202	C2E	O21-P11-O3'	2.82	117.82	106.49
2	B	203	C2E	C3'-C2'-C1'	2.83	106.30	99.95
2	B	201	C2E	C2A-C3A-C4A	2.86	108.36	103.23
2	A	202	C2E	N2-C2-N1	2.87	121.83	117.24
2	D	203	C2E	C3A-C2A-C1A	2.87	106.40	99.95
2	D	202	C2E	C61-N11-C21	2.89	120.21	116.06
2	B	202	C2E	C6-N1-C2	2.91	120.24	116.06
2	B	201	C2E	O21-P11-O3'	2.92	118.22	106.49
2	A	202	C2E	C3A-C2A-C1A	2.92	106.52	99.95
2	A	201	C2E	C61-N11-C21	2.94	120.29	116.06
2	B	202	C2E	C2-N3-C4	2.97	118.63	115.16
2	C	203	C2E	C2-N3-C4	3.00	118.67	115.16
2	A	203	C2E	N21-C21-N11	3.03	122.08	117.24
2	C	203	C2E	C3'-C2'-C1'	3.05	106.79	99.95
2	D	202	C2E	O21-P11-O3'	3.05	118.74	106.49
2	C	202	C2E	C1A-N91-C41	3.05	131.91	126.64
2	D	201	C2E	C6-N1-C2	3.06	120.46	116.06
2	C	201	C2E	C6-N1-C2	3.07	120.47	116.06
2	D	203	C2E	C6-N1-C2	3.07	120.47	116.06
2	C	202	C2E	O2P-P1-O3A	3.14	119.09	106.49
2	C	202	C2E	C6-N1-C2	3.20	120.66	116.06
2	D	203	C2E	N2-C2-N1	3.20	122.36	117.24
2	A	201	C2E	O21-P11-O3'	3.20	119.36	106.49
2	B	202	C2E	C3A-C2A-C1A	3.27	107.28	99.95
2	A	203	C2E	C1A-N91-C41	3.29	132.33	126.64
2	C	201	C2E	O21-P11-O3'	3.36	119.97	106.49
2	D	202	C2E	C21-N31-C41	3.37	119.09	115.16
2	D	201	C2E	N2-C2-N1	3.37	122.63	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	202	C2E	C21-N31-C41	3.38	119.11	115.16
2	A	202	C2E	C2-N3-C4	3.39	119.12	115.16
2	D	201	C2E	C2-N3-C4	3.39	119.12	115.16
2	A	203	C2E	O21-P11-O3'	3.43	120.29	106.49
2	B	203	C2E	C21-N31-C41	3.46	119.20	115.16
2	C	203	C2E	C6-N1-C2	3.49	121.08	116.06
2	D	202	C2E	C2-N3-C4	3.51	119.26	115.16
2	D	203	C2E	C3'-C2'-C1'	3.52	107.85	99.95
2	A	201	C2E	C2-N3-C4	3.53	119.28	115.16
2	B	201	C2E	C1A-N91-C41	3.58	132.82	126.64
2	D	201	C2E	N21-C21-N11	3.60	122.99	117.24
2	A	203	C2E	C2-N3-C4	3.74	119.53	115.16
2	B	201	C2E	C6-N1-C2	3.79	121.52	116.06
2	A	203	C2E	C21-N31-C41	3.80	119.59	115.16
2	C	201	C2E	C1A-N91-C41	3.84	133.27	126.64
2	B	201	C2E	C21-N31-C41	3.94	119.76	115.16
2	D	203	C2E	C21-N31-C41	3.95	119.78	115.16
2	D	203	C2E	C2-N3-C4	3.97	119.79	115.16
2	A	201	C2E	C1A-N91-C41	3.98	133.51	126.64
2	C	203	C2E	C21-N31-C41	4.00	119.83	115.16
2	A	202	C2E	C21-N31-C41	4.01	119.84	115.16
2	D	202	C2E	C1A-N91-C41	4.13	133.77	126.64
2	C	201	C2E	C21-N31-C41	4.18	120.05	115.16
2	D	203	C2E	C1A-N91-C41	4.22	133.93	126.64
2	A	201	C2E	C21-N31-C41	4.26	120.13	115.16
2	B	203	C2E	C1A-N91-C41	4.27	134.02	126.64
2	B	202	C2E	C21-N31-C41	4.29	120.17	115.16
2	B	203	C2E	C2-N3-C4	4.35	120.24	115.16
2	A	202	C2E	C1A-N91-C41	4.55	134.50	126.64
2	B	202	C2E	C1A-N91-C41	4.68	134.71	126.64
2	D	201	C2E	C21-N31-C41	5.61	121.71	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	C2E	1	0
2	A	202	C2E	5	0
2	B	201	C2E	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	202	C2E	1	0
2	C	203	C2E	1	0
2	D	203	C2E	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	104/111 (93%)	0.02	2 (1%)	67	66	22, 37, 58, 68	0
1	B	103/111 (92%)	-0.03	2 (1%)	67	66	23, 35, 55, 68	0
1	C	108/111 (97%)	0.32	11 (10%)	7	8	20, 38, 66, 94	0
1	D	106/111 (95%)	0.11	4 (3%)	41	41	19, 35, 59, 70	0
All	All	421/444 (94%)	0.11	19 (4%)	34	34	19, 36, 60, 94	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	24	ARG	5.8
1	C	23	ASN	3.7
1	A	3	GLY	3.7
1	C	21	GLY	3.7
1	C	109	ALA	3.3
1	C	67	PHE	3.3
1	A	62	VAL	3.1
1	C	22	ALA	2.8
1	B	22	ALA	2.8
1	D	1	GLY	2.8
1	C	25	GLU	2.7
1	D	4	SER	2.6
1	C	20	ILE	2.6
1	D	23	ASN	2.4
1	C	62	VAL	2.4
1	C	60	PHE	2.2
1	B	24	ARG	2.2
1	C	94	PRO	2.2
1	D	102	TYR	2.1

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

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

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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	C2E	C	202	46/46	0.96	0.12	0.78	17,21,23,24	0
2	C2E	C	201	46/46	0.96	0.12	0.03	17,22,26,28	0
2	C2E	B	202	46/46	0.95	0.13	-0.00	25,30,34,36	0
2	C2E	B	201	46/46	0.92	0.12	-0.09	22,31,38,39	0
2	C2E	D	201	46/46	0.96	0.11	-0.12	20,24,28,31	0
2	C2E	D	202	46/46	0.94	0.12	-0.18	19,27,31,34	0
2	C2E	A	202	46/46	0.91	0.14	-0.23	28,33,38,43	0
2	C2E	A	201	46/46	0.93	0.10	-0.40	24,32,38,42	0
2	C2E	C	203	46/46	0.96	0.11	-0.50	18,25,31,35	0
2	C2E	D	203	46/46	0.93	0.14	-1.09	22,31,39,44	0
3	ZN	A	205	1/1	1.00	0.09	-1.90	29,29,29,29	1
3	ZN	B	208	1/1	1.00	0.09	-1.99	25,25,25,25	1
3	ZN	B	205	1/1	0.99	0.12	-	30,30,30,30	0
3	ZN	A	204	1/1	1.00	0.06	-	29,29,29,29	1
2	C2E	B	203	46/46	0.93	0.12	-	20,28,35,38	0
3	ZN	B	206	1/1	0.99	0.12	-	26,26,26,26	0
3	ZN	B	207	1/1	0.95	0.08	-	49,49,49,49	0
2	C2E	A	203	46/46	0.93	0.13	-	26,32,40,43	0
3	ZN	C	204	1/1	1.00	0.09	-	23,23,23,23	1
3	ZN	B	204	1/1	1.00	0.08	-	22,22,22,22	1
3	ZN	D	204	1/1	0.99	0.06	-	22,22,22,22	1
3	ZN	D	205	1/1	0.93	0.14	-	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.