WORLD WIDE
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 22, 2025 – 12:38 AM EDT

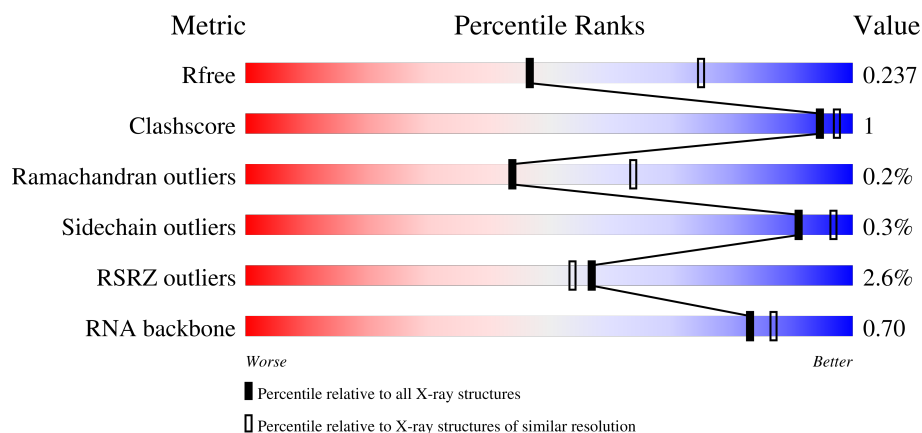|		
PDB ID	:	4X4T / pdb_00004x4t
Title	:	Crystal structure of the A.fulgidus CCA-adding enzyme in complex with a G70A arginyl-tRNA minihelix ending in CCACCA
Authors	:	Kuhn, C.-D.; Joshua-Tor, L.
Deposited on	:	2014-12-03
Resolution	:	2.50 Å(reported)

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 2.50 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		0.237
Clashscore		1
Ramachandran outliers		0.2%
Sidechain outliers		0.3%
RSRZ outliers		2.6%
RNA backbone		0.70

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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)
RNA backbone	3690	1181 (2.80-2.20)

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	457	3% / 92% · ·
1	C	457	4% / 94% · ·
1	E	457	% / 93% · ·
1	F	457	% / 92% · ·

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Mol	Chain	Length	Quality of chain
2	B	34	76% 24%
2	D	34	65% 18% · · 12%
3	G	33	6% 45% 15% 39%
4	H	2	50% 50%
5	I	2	100% 50% 50%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 32835 atoms, of which 15704 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 CCA-adding enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			7270	2333	3641	632	651	13			
1	C	437	Total	C	H	N	O	S	0	0	0
			7265	2333	3637	631	651	13			
1	E	437	Total	C	H	N	O	S	0	0	0
			7270	2333	3641	632	651	13			
1	F	437	Total	C	H	N	O	S	0	0	0
			7270	2333	3641	632	651	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	SER	-	expression tag	UNP O28126
A	439	ASN	-	expression tag	UNP O28126
A	440	SER	-	expression tag	UNP O28126
A	441	SER	-	expression tag	UNP O28126
A	442	SER	-	expression tag	UNP O28126
A	443	VAL	-	expression tag	UNP O28126
A	444	ASP	-	expression tag	UNP O28126
A	445	LYS	-	expression tag	UNP O28126
A	446	LEU	-	expression tag	UNP O28126
A	447	ALA	-	expression tag	UNP O28126
A	448	ALA	-	expression tag	UNP O28126
A	449	ALA	-	expression tag	UNP O28126
A	450	LEU	-	expression tag	UNP O28126
A	451	GLU	-	expression tag	UNP O28126
A	452	HIS	-	expression tag	UNP O28126
A	453	HIS	-	expression tag	UNP O28126
A	454	HIS	-	expression tag	UNP O28126
A	455	HIS	-	expression tag	UNP O28126
A	456	HIS	-	expression tag	UNP O28126
A	457	HIS	-	expression tag	UNP O28126
C	438	SER	-	expression tag	UNP O28126

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Chain	Residue	Modelled	Actual	Comment	Reference
C	439	ASN	-	expression tag	UNP O28126
C	440	SER	-	expression tag	UNP O28126
C	441	SER	-	expression tag	UNP O28126
C	442	SER	-	expression tag	UNP O28126
C	443	VAL	-	expression tag	UNP O28126
C	444	ASP	-	expression tag	UNP O28126
C	445	LYS	-	expression tag	UNP O28126
C	446	LEU	-	expression tag	UNP O28126
C	447	ALA	-	expression tag	UNP O28126
C	448	ALA	-	expression tag	UNP O28126
C	449	ALA	-	expression tag	UNP O28126
C	450	LEU	-	expression tag	UNP O28126
C	451	GLU	-	expression tag	UNP O28126
C	452	HIS	-	expression tag	UNP O28126
C	453	HIS	-	expression tag	UNP O28126
C	454	HIS	-	expression tag	UNP O28126
C	455	HIS	-	expression tag	UNP O28126
C	456	HIS	-	expression tag	UNP O28126
C	457	HIS	-	expression tag	UNP O28126
E	438	SER	-	expression tag	UNP O28126
E	439	ASN	-	expression tag	UNP O28126
E	440	SER	-	expression tag	UNP O28126
E	441	SER	-	expression tag	UNP O28126
E	442	SER	-	expression tag	UNP O28126
E	443	VAL	-	expression tag	UNP O28126
E	444	ASP	-	expression tag	UNP O28126
E	445	LYS	-	expression tag	UNP O28126
E	446	LEU	-	expression tag	UNP O28126
E	447	ALA	-	expression tag	UNP O28126
E	448	ALA	-	expression tag	UNP O28126
E	449	ALA	-	expression tag	UNP O28126
E	450	LEU	-	expression tag	UNP O28126
E	451	GLU	-	expression tag	UNP O28126
E	452	HIS	-	expression tag	UNP O28126
E	453	HIS	-	expression tag	UNP O28126
E	454	HIS	-	expression tag	UNP O28126
E	455	HIS	-	expression tag	UNP O28126
E	456	HIS	-	expression tag	UNP O28126
E	457	HIS	-	expression tag	UNP O28126
F	438	SER	-	expression tag	UNP O28126
F	439	ASN	-	expression tag	UNP O28126
F	440	SER	-	expression tag	UNP O28126

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Chain	Residue	Modelled	Actual	Comment	Reference
F	441	SER	-	expression tag	UNP O28126
F	442	SER	-	expression tag	UNP O28126
F	443	VAL	-	expression tag	UNP O28126
F	444	ASP	-	expression tag	UNP O28126
F	445	LYS	-	expression tag	UNP O28126
F	446	LEU	-	expression tag	UNP O28126
F	447	ALA	-	expression tag	UNP O28126
F	448	ALA	-	expression tag	UNP O28126
F	449	ALA	-	expression tag	UNP O28126
F	450	LEU	-	expression tag	UNP O28126
F	451	GLU	-	expression tag	UNP O28126
F	452	HIS	-	expression tag	UNP O28126
F	453	HIS	-	expression tag	UNP O28126
F	454	HIS	-	expression tag	UNP O28126
F	455	HIS	-	expression tag	UNP O28126
F	456	HIS	-	expression tag	UNP O28126
F	457	HIS	-	expression tag	UNP O28126

- Molecule 2 is a RNA chain called G70A tRNA minihelix ending in CCACCA.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	34	Total	Br	C	H	N	O	P	0	6	0
			1083	3	322	355	129	240	34			
2	D	30	Total	Br	C	H	N	O	P	0	0	0
			968	2	284	325	114	213	30			

- Molecule 3 is a RNA chain called G70A tRNA minihelix ending in CCACCA.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
3	G	18	Total	Br	C	H	N	O	P	0	18	0
			1159	1	342	385	143	252	36			

- Molecule 4 is a RNA chain called RNA (5'-D(P*CP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	2	Total	C	H	N	O	P	0	0	0
			66	19	23	8	14	2			

- Molecule 5 is a RNA chain called RNA (5'-D(P*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
5	I	2	68	20	22	10	14	2	0	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).
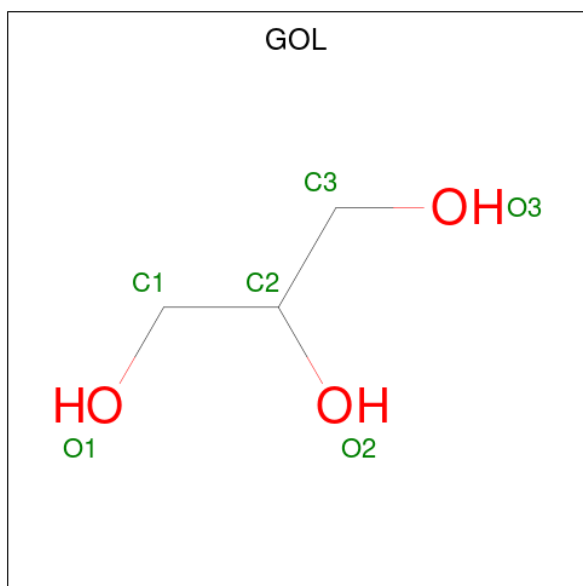
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).
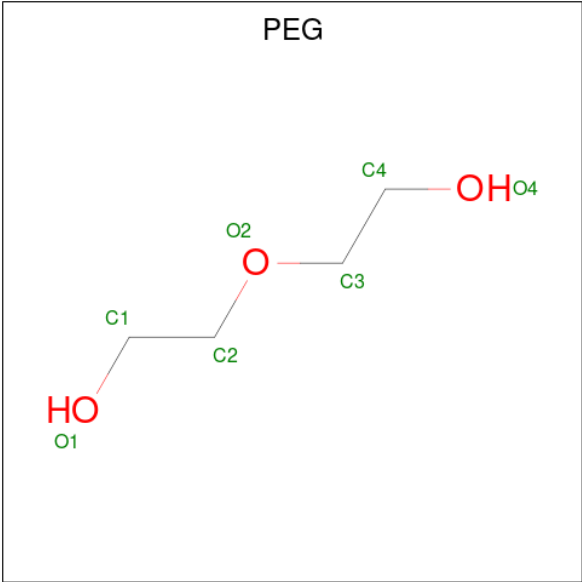
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	E	1	17	4	10	3	0	0

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	63	Total 63	O 63	0	0
8	B	2	Total 2	O 2	0	0
8	C	51	Total 51	O 51	0	0
8	E	133	Total 133	O 133	0	0
8	F	96	Total 96	O 96	0	0
8	G	12	Total 12	O 12	0	0

3 Residue-property plots ⓘ

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: CCA-adding enzyme
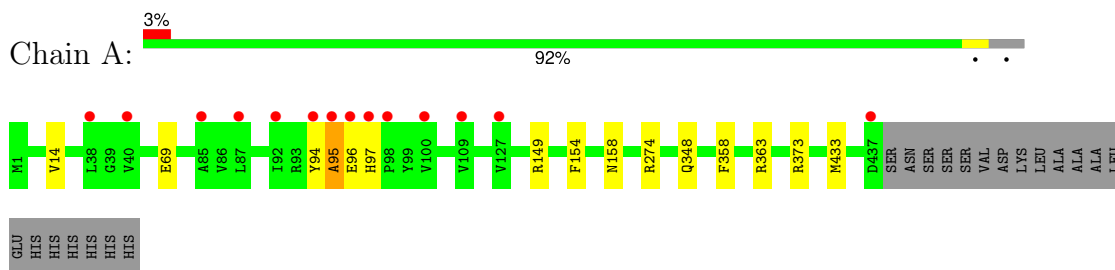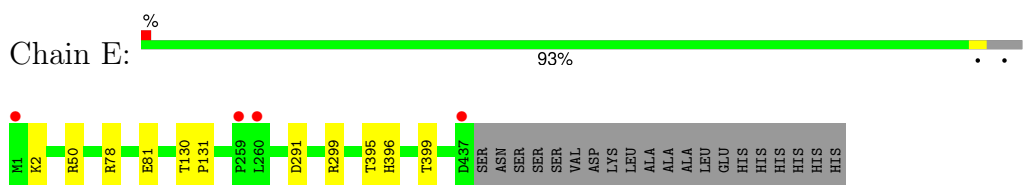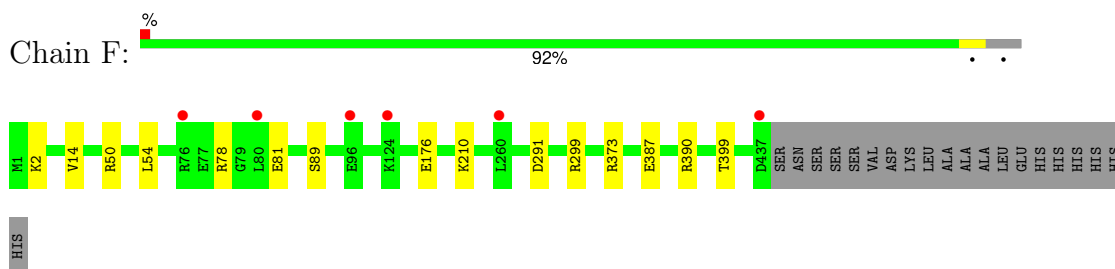

- Molecule 1: CCA-adding enzyme
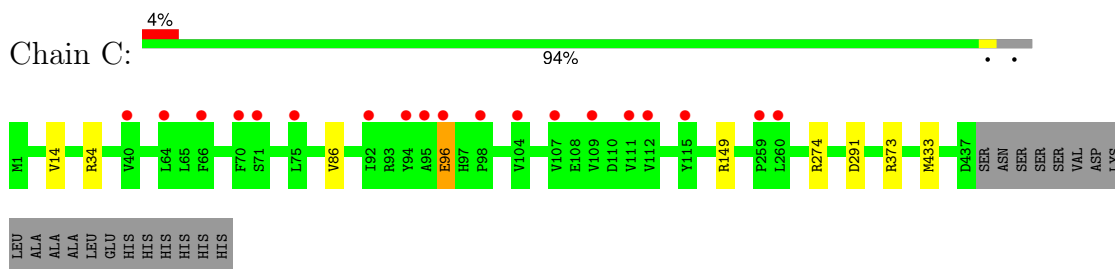
- Molecule 1: CCA-adding enzyme

- Molecule 1: CCA-adding enzyme

- Molecule 2: G70A tRNA minihelix ending in CCACCA

Chain B:
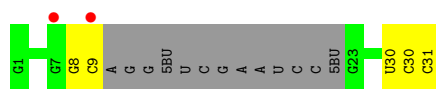

• Molecule 2: G70A tRNA minihelix ending in CCACCA

Chain D:

• Molecule 3: G70A tRNA minihelix ending in CCACCA

Chain G:

• Molecule 4: RNA (5'-D(P*CP*G)-3')

Chain H:

• Molecule 5: RNA (5'-D(P*GP*G)-3')

Chain I:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.42Å 83.96Å 135.32Å 90.00° 103.51° 90.00°	Depositor
Resolution (Å)	39.34 – 2.50	Depositor
	39.34 – 2.50	EDS
% Data completeness	99.3 (39.34-2.50)	Depositor
(in resolution range)	100.0 (39.34-2.50)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.186 , 0.229	Depositor
	0.194 , 0.237	DCC
R_{free} test set	4370 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32835	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5BU, PEG, GOL

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	0.23	0/3712	0.39	0/4987
1	C	0.23	0/3711	0.39	0/4985
1	E	0.24	0/3712	0.39	0/4987
1	F	0.23	0/3712	0.40	0/4987
2	B	0.42	1/741 (0.1%)	0.68	1/1150 (0.1%)
2	D	0.45	1/669 (0.1%)	0.72	1/1038 (0.1%)
3	G	0.15	0/834	0.67	0/1286
4	H	0.13	0/47	0.64	0/71
5	I	0.20	0/51	0.77	0/78
All	All	0.25	2/17189 (0.0%)	0.45	2/23569 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-10.60	1.48	1.61
2	D	1	G	OP3-P	-10.55	1.48	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	G	OP1-P-O3'	5.27	116.79	105.20
2	B	1	G	OP1-P-O3'	5.16	116.55	105.20

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	3629	3641	3633	8	0
1	C	3628	3637	3629	5	0
1	E	3629	3641	3633	7	0
1	F	3629	3641	3633	10	0
2	B	728	355	365	2	0
2	D	643	325	324	5	0
3	G	774	385	397	3	0
4	H	43	23	23	1	0
5	I	46	22	23	2	0
6	A	18	24	24	0	0
7	E	7	10	9	0	0
8	A	63	0	0	0	0
8	B	2	0	0	0	0
8	C	51	0	0	0	0
8	E	133	0	0	1	0
8	F	96	0	0	4	0
8	G	12	0	0	0	0
All	All	17131	15704	15693	36	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 1.

The worst 5 of 36 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:B:19:U:H3	5:I:1:G:HO2'	1.27	0.76
1:F:299:ARG:NH1	1:F:399:THR:O	2.23	0.72
1:A:274:ARG:NH2	1:A:433:MET:O	2.24	0.71
2:B:17:A:O2'	2:B:19:U:OP2	2.11	0.68
1:A:358:PHE:O	1:A:363:ARG:NH2	2.26	0.67

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/457 (95%)	416 (96%)	18 (4%)	1 (0%)	44	64
1	C	435/457 (95%)	412 (95%)	22 (5%)	1 (0%)	44	64
1	E	435/457 (95%)	425 (98%)	10 (2%)	0	100	100
1	F	435/457 (95%)	425 (98%)	9 (2%)	1 (0%)	44	64
All	All	1740/1828 (95%)	1678 (96%)	59 (3%)	3 (0%)	44	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ALA
1	C	96	GLU
1	F	2	LYS

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	387/404 (96%)	386 (100%)	1 (0%)	91	97
1	C	386/404 (96%)	385 (100%)	1 (0%)	91	97
1	E	387/404 (96%)	386 (100%)	1 (0%)	91	97
1	F	387/404 (96%)	386 (100%)	1 (0%)	91	97
All	All	1547/1616 (96%)	1543 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	C	96	GLU
1	E	2	LYS
1	F	89	SER

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

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	32/34 (94%)	2 (6%)	0
2	D	28/34 (82%)	3 (10%)	0
3	G	1/33 (3%)	0	0
4	H	1/2 (50%)	0	0
5	I	1/2 (50%)	1 (100%)	0
All	All	63/105 (60%)	6 (9%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	18	A
2	B	20	C
2	D	2	G
2	D	22	5BU
2	D	26	G

There are no RNA pucker outliers to report.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	5BU	B	22	2	19,22,23	3.88	5 (26%)	27,32,35	3.53	10 (37%)
2	5BU	B	30[B]	2	19,22,23	3.89	5 (26%)	27,32,35	3.52	9 (33%)
2	5BU	D	22	2	19,22,23	3.89	5 (26%)	27,32,35	3.57	9 (33%)
2	5BU	D	13	2	19,22,23	3.89	5 (26%)	27,32,35	3.54	9 (33%)
2	5BU	B	13	2	19,22,23	3.89	5 (26%)	27,32,35	3.54	10 (37%)
3	5BU	G	30[A]	3	19,22,23	3.91	5 (26%)	27,32,35	3.48	9 (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
2	5BU	B	22	2	-	0/7/25/26	0/2/2/2
2	5BU	B	30[B]	2	-	0/7/25/26	0/2/2/2
2	5BU	D	22	2	-	2/7/25/26	0/2/2/2
2	5BU	D	13	2	-	0/7/25/26	0/2/2/2
2	5BU	B	13	2	-	0/7/25/26	0/2/2/2
3	5BU	G	30[A]	3	-	0/7/25/26	0/2/2/2

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	30[A]	5BU	C6-N1	12.64	1.59	1.38
2	D	13	5BU	C6-N1	12.55	1.59	1.38
2	B	13	5BU	C6-N1	12.54	1.59	1.38
2	B	30[B]	5BU	C6-N1	12.54	1.59	1.38
2	D	22	5BU	C6-N1	12.53	1.59	1.38

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	22	5BU	C5-C4-N3	9.69	124.49	113.34
2	D	13	5BU	C5-C4-N3	9.67	124.46	113.34
2	B	13	5BU	C5-C4-N3	9.65	124.44	113.34
2	D	22	5BU	C5-C4-N3	9.64	124.43	113.34
2	B	30[B]	5BU	C5-C4-N3	9.57	124.35	113.34

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	22	5BU	O4'-C4'-C5'-O5'
2	D	22	5BU	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	22	5BU	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
6	GOL	A	502	-	5,5,5	0.37	0	5,5,5	0.24	0
6	GOL	A	503	-	5,5,5	0.38	0	5,5,5	0.24	0
6	GOL	A	501	-	5,5,5	0.35	0	5,5,5	0.27	0
7	PEG	E	501	-	6,6,6	0.61	0	5,5,5	0.26	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	502	-	-	1/4/4/4	-
6	GOL	A	503	-	-	2/4/4/4	-
6	GOL	A	501	-	-	2/4/4/4	-
7	PEG	E	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	GOL	O1-C1-C2-C3
6	A	503	GOL	O1-C1-C2-C3
6	A	501	GOL	O1-C1-C2-O2
6	A	503	GOL	O1-C1-C2-O2
6	A	502	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	437/457 (95%)	0.00	14 (3%)	50	47	33, 64, 152, 180	0
1	C	437/457 (95%)	0.18	19 (4%)	40	37	34, 70, 167, 225	0
1	E	437/457 (95%)	-0.41	4 (0%)	81	78	31, 52, 97, 141	0
1	F	437/457 (95%)	-0.30	6 (1%)	73	70	37, 54, 97, 154	0
2	B	31/34 (91%)	0.79	0	100	100	30, 136, 206, 215	5 (16%)
2	D	28/34 (82%)	0.85	0	100	100	96, 154, 200, 214	0
3	G	16/33 (48%)	0.61	2 (12%)	9	9	26, 31, 51, 51	16 (100%)
4	H	2/2 (100%)	1.33	0	100	100	91, 91, 91, 112	0
5	I	2/2 (100%)	2.49	2 (100%)	0	0	98, 98, 98, 168	0
All	All	1827/1933 (94%)	-0.09	47 (2%)	57	54	26, 59, 156, 225	21 (1%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	ALA	4.0
1	A	95	ALA	3.4
1	C	40	VAL	3.4
1	A	96	GLU	3.2
1	F	437	ASP	3.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	5BU	D	22	21/22	0.70	0.14	151,160,190,197	0
2	5BU	B	22	21/22	0.71	0.14	134,145,171,184	0
2	5BU	B	30[B]	21/22	0.83	0.13	80,89,106,107	30
2	5BU	D	13	21/22	0.84	0.10	121,145,166,180	0
2	5BU	B	13	21/22	0.84	0.10	109,129,151,160	0
3	5BU	G	30[A]	21/22	0.91	0.11	41,44,56,108	30

6.3 Carbohydrates ⓘ

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
6	GOL	A	502	6/6	0.75	0.22	59,71,75,75	0
6	GOL	A	501	6/6	0.80	0.16	80,96,105,106	0
7	PEG	E	501	7/7	0.87	0.20	75,95,118,119	0
6	GOL	A	503	6/6	0.89	0.16	70,84,92,95	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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