Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2023 – 08:47 PM EDT

PDB ID	:	1RBY
Title	:	Human GAR Tfase complex structure with 10-(trifluoroacetyl)-5,10-dideazaa cyclic-5,6,7,8-tetrahydrofolic acid and substrate beta-GAR
Authors	:	Zhang, Y.; Desharnais, J.; Boger, D.L.; Wilson, I.A.
Deposited on	:	2003-11-03
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

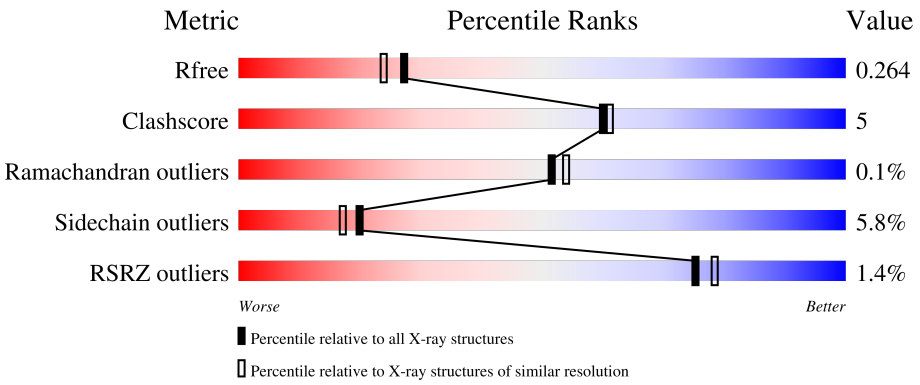
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	209	.% 83% 11% • •
1	B	209	82% 11% • •
1	C	209	2% 85% 9% • •
1	D	209	.% 85% 9% • •

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
2	KEU	A	510	X	-	-	-
2	KEU	B	610	X	-	-	-
2	KEU	C	710	X	-	-	-
2	KEU	D	810	X	-	-	-
3	GAR	A	523	X	-	X	-
3	GAR	B	623	X	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6727 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 PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1507	954	264	284	5	0	0	0
1	B	200	1507	954	264	284	5	0	0	0
1	C	200	1507	954	264	284	5	0	0	0
1	D	200	1507	954	264	284	5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	HIS	-	expression tag	UNP P22102
A	205	HIS	-	expression tag	UNP P22102
A	206	HIS	-	expression tag	UNP P22102
A	207	HIS	-	expression tag	UNP P22102
A	208	HIS	-	expression tag	UNP P22102
A	209	HIS	-	expression tag	UNP P22102
B	204	HIS	-	expression tag	UNP P22102
B	205	HIS	-	expression tag	UNP P22102
B	206	HIS	-	expression tag	UNP P22102
B	207	HIS	-	expression tag	UNP P22102
B	208	HIS	-	expression tag	UNP P22102
B	209	HIS	-	expression tag	UNP P22102
C	204	HIS	-	expression tag	UNP P22102
C	205	HIS	-	expression tag	UNP P22102
C	206	HIS	-	expression tag	UNP P22102
C	207	HIS	-	expression tag	UNP P22102
C	208	HIS	-	expression tag	UNP P22102
C	209	HIS	-	expression tag	UNP P22102
D	204	HIS	-	expression tag	UNP P22102
D	205	HIS	-	expression tag	UNP P22102

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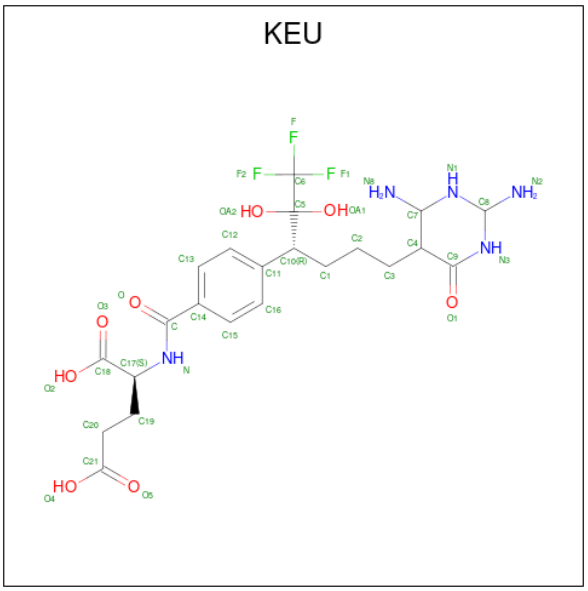
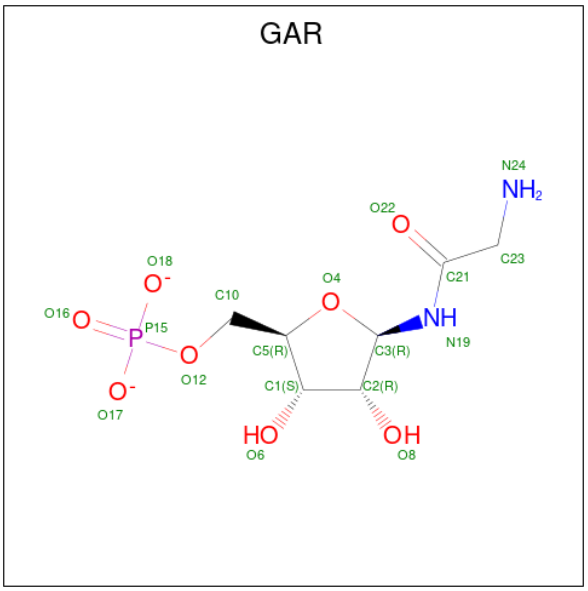
Chain	Residue	Modelled	Actual	Comment	Reference
D	206	HIS	-	expression tag	UNP P22102
D	207	HIS	-	expression tag	UNP P22102
D	208	HIS	-	expression tag	UNP P22102
D	209	HIS	-	expression tag	UNP P22102

- Molecule 2 is N-{4-[(1R)-4-[(2R,4R,5S)-2,4-DIAMINO-6-OXOHEXAHYDROPYRIMIDIN-5-YL]-1-(2,2,2-TRIFLUORO-1,1-DIHYDROXYETHYL)BUTYL]BENZOYL}-D-GLUTAMIC ACID (three-letter code: KEU) (formula: $C_{22}H_{30}F_3N_5O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	38	22	3	5	8	0	0
			Total	C	F	N	O		
2	B	1	38	22	3	5	8	0	0
			Total	C	F	N	O		
2	C	1	38	22	3	5	8	0	0
			Total	C	F	N	O		
2	D	1	38	22	3	5	8	0	0

- Molecule 3 is GLYCINAMIDE RIBONUCLEOTIDE (three-letter code: GAR) (formula: $C_7H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	18	7	2	8	1	0	0
			Total	C	N	O	P		
3	B	1	18	7	2	8	1	0	0

- Molecule 4 is water.

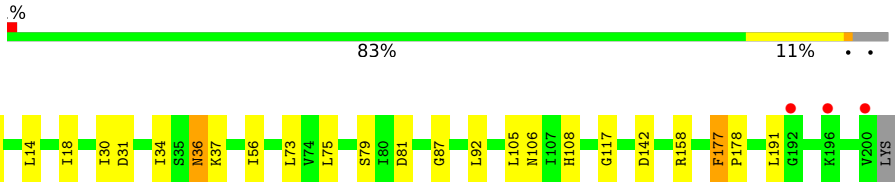
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	150	150	150	0	0
			Total	O		
4	B	133	133	133	0	0
			Total	O		
4	C	112	112	112	0	0
			Total	O		
4	D	116	116	116	0	0

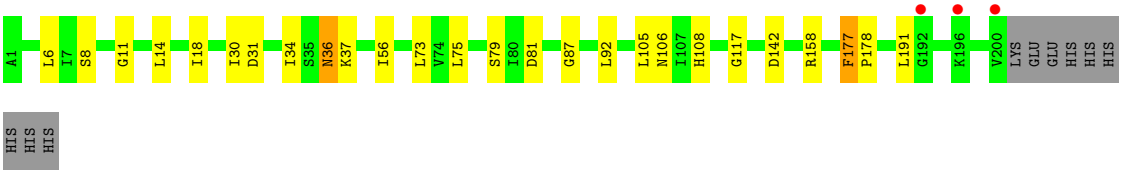
3 Residue-property plots (i)

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: PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE

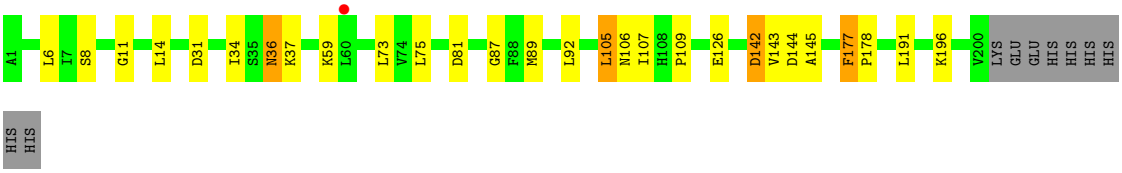
Chain A:





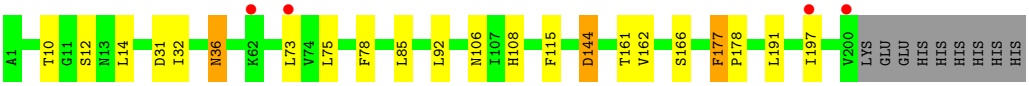
• Molecule 1: PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE

Chain B:



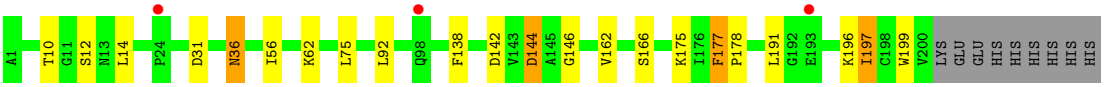
• Molecule 1: PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE

Chain C:



• Molecule 1: PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	126.17Å 126.17Å 95.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.67 – 2.10 47.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (47.67-2.10) 93.9 (47.41-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.245 , 0.264 0.245 , 0.264	Depositor DCC
R_{free} test set	4693 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.438 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6727	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GAR, KEU

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	0.56	0/1530	0.71	2/2076 (0.1%)
1	B	0.53	0/1530	0.69	3/2076 (0.1%)
1	C	0.53	0/1530	0.69	2/2076 (0.1%)
1	D	0.49	0/1530	0.70	3/2076 (0.1%)
All	All	0.53	0/6120	0.70	10/8304 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	144	ASP	CB-CG-OD2	6.08	123.77	118.30
1	D	31	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	105	LEU	CA-CB-CG	5.83	128.72	115.30
1	B	31	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	81	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	81	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	31	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	142	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	31	ASP	CB-CG-OD2	5.06	122.86	118.30
1	D	144	ASP	CB-CG-OD2	5.04	122.83	118.30

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	1507	0	1548	16	0
1	B	1507	0	1548	20	0
1	C	1507	0	1548	10	0
1	D	1507	0	1548	11	0
2	A	38	0	24	2	0
2	B	38	0	25	4	0
2	C	38	0	25	3	0
2	D	38	0	25	2	0
3	A	18	0	13	7	0
3	B	18	0	13	11	0
4	A	150	0	0	2	0
4	B	133	0	0	1	0
4	C	112	0	0	0	0
4	D	116	0	0	2	0
All	All	6727	0	6317	57	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 5.

All (57) 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:C:92:LEU:H	2:C:710:KEU:HN1	1.22	0.86
1:D:92:LEU:H	2:D:810:KEU:HN1	1.29	0.81
1:B:92:LEU:H	2:B:610:KEU:HN1	1.29	0.81
1:B:87:GLY:H	3:B:623:GAR:C21	1.96	0.79
1:A:92:LEU:H	2:A:510:KEU:HN1	1.28	0.78
1:B:144:ASP:OD1	2:B:610:KEU:H12A	1.95	0.67
1:A:87:GLY:HA2	3:A:523:GAR:C21	2.26	0.64
1:B:107:ILE:HG23	3:B:623:GAR:H19	1.62	0.63
1:B:106:ASN:OD1	3:B:623:GAR:C23	2.46	0.63
1:B:87:GLY:HA2	3:B:623:GAR:C21	2.30	0.62
1:A:87:GLY:H	3:A:523:GAR:C21	2.14	0.61
1:B:87:GLY:N	3:B:623:GAR:C21	2.63	0.61
1:C:144:ASP:OD1	2:C:710:KEU:H12A	2.00	0.60
1:D:162:VAL:O	1:D:166:SER:HB2	2.02	0.59
1:B:87:GLY:CA	3:B:623:GAR:C21	2.83	0.56
1:B:106:ASN:OD1	3:B:623:GAR:H231	2.06	0.56
1:B:177:PHE:HB3	1:B:178:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:HIS:HD2	2:C:710:KEU:OA2	1.89	0.55
1:D:144:ASP:OD1	2:D:810:KEU:H12A	2.09	0.53
1:A:87:GLY:CA	3:A:523:GAR:C21	2.87	0.53
1:A:11:GLY:HA2	4:A:574:HOH:O	2.08	0.53
1:A:6:LEU:HD22	1:A:34:ILE:HB	1.91	0.52
1:C:162:VAL:O	1:C:166:SER:HB2	2.09	0.52
1:D:175:LYS:HE3	4:D:848:HOH:O	2.10	0.51
1:C:36:ASN:HD22	1:C:36:ASN:H	1.58	0.51
1:D:177:PHE:HB3	1:D:178:PRO:HD3	1.93	0.50
1:A:106:ASN:OD1	3:A:523:GAR:C23	2.59	0.50
1:A:177:PHE:HB3	1:A:178:PRO:HD3	1.94	0.50
2:A:510:KEU:F1	3:A:523:GAR:O22	2.20	0.50
1:B:6:LEU:HD22	1:B:34:ILE:HB	1.93	0.50
1:D:138:PHE:O	1:D:146:GLY:HA3	2.11	0.50
1:D:36:ASN:HD22	1:D:36:ASN:H	1.59	0.49
1:C:85:LEU:HB2	1:C:106:ASN:HD22	1.78	0.49
1:A:106:ASN:OD1	3:A:523:GAR:H231	2.11	0.49
1:A:8:SER:OG	1:A:36:ASN:ND2	2.45	0.48
1:B:89:MET:CE	3:B:623:GAR:O22	2.61	0.48
4:A:661:HOH:O	1:D:196:LYS:HE3	2.13	0.48
1:B:142:ASP:HB3	1:B:145:ALA:HB3	1.95	0.47
1:C:108:HIS:HE1	1:C:115:PHE:O	1.97	0.47
1:C:32:ILE:HD13	1:C:78:PHE:CZ	2.50	0.47
1:A:36:ASN:HA	1:A:56:ILE:O	2.15	0.46
1:A:87:GLY:N	3:A:523:GAR:C21	2.78	0.46
1:C:177:PHE:HB3	1:C:178:PRO:HD3	1.97	0.46
1:B:126:GLU:OE1	1:C:161:THR:HB	2.16	0.45
1:B:89:MET:HE1	3:B:623:GAR:O22	2.16	0.45
1:A:36:ASN:H	1:A:36:ASN:HD22	1.63	0.45
1:B:109:PRO:HD3	3:B:623:GAR:O8	2.18	0.44
1:B:11:GLY:HA2	4:B:650:HOH:O	2.17	0.44
1:B:36:ASN:H	1:B:36:ASN:HD22	1.66	0.43
1:D:197:ILE:HG21	4:D:837:HOH:O	2.19	0.43
1:A:158:ARG:HD3	1:D:199:TRP:CD1	2.54	0.42
1:B:143:VAL:HG13	2:B:610:KEU:H11	2.01	0.42
1:B:8:SER:OG	1:B:36:ASN:ND2	2.49	0.42
1:A:108:HIS:HE1	1:A:117:GLY:O	2.04	0.41
1:D:36:ASN:HA	1:D:56:ILE:O	2.21	0.41
1:A:18:ILE:HA	1:A:30:ILE:HD12	2.03	0.40
2:B:610:KEU:F1	3:B:623:GAR:O22	2.29	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	198/209 (95%)	192 (97%)	5 (2%)	1 (0%)	29	26
1	B	198/209 (95%)	194 (98%)	4 (2%)	0	100	100
1	C	198/209 (95%)	196 (99%)	2 (1%)	0	100	100
1	D	198/209 (95%)	194 (98%)	4 (2%)	0	100	100
All	All	792/836 (95%)	776 (98%)	15 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	SER

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	164/173 (95%)	155 (94%)	9 (6%)	21	19
1	B	164/173 (95%)	153 (93%)	11 (7%)	16	13
1	C	164/173 (95%)	155 (94%)	9 (6%)	21	19
1	D	164/173 (95%)	155 (94%)	9 (6%)	21	19
All	All	656/692 (95%)	618 (94%)	38 (6%)	20	17

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	36	ASN
1	A	37	LYS
1	A	73	LEU
1	A	75	LEU
1	A	105	LEU
1	A	142	ASP
1	A	177	PHE
1	A	191	LEU
1	B	14	LEU
1	B	36	ASN
1	B	37	LYS
1	B	59	LYS
1	B	73	LEU
1	B	75	LEU
1	B	105	LEU
1	B	142	ASP
1	B	177	PHE
1	B	191	LEU
1	B	196	LYS
1	C	10	THR
1	C	12	SER
1	C	14	LEU
1	C	36	ASN
1	C	73	LEU
1	C	75	LEU
1	C	177	PHE
1	C	191	LEU
1	C	197	ILE
1	D	10	THR
1	D	12	SER
1	D	14	LEU
1	D	36	ASN
1	D	62	LYS
1	D	75	LEU
1	D	177	PHE
1	D	191	LEU
1	D	197	ILE

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	36	ASN

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Mol	Chain	Res	Type
1	B	36	ASN
1	C	36	ASN
1	C	106	ASN
1	C	108	HIS
1	D	36	ASN
1	D	98	GLN
1	D	147	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
2	KEU	C	710	-	34,39,39	7.16	17 (50%)	41,57,57	4.63	19 (46%)
2	KEU	A	510	-	34,39,39	6.99	17 (50%)	41,57,57	4.80	18 (43%)
2	KEU	B	610	-	34,39,39	6.99	16 (47%)	41,57,57	4.51	20 (48%)
3	GAR	A	523	-	17,18,18	3.58	6 (35%)	21,26,26	2.00	3 (14%)
2	KEU	D	810	-	34,39,39	7.26	18 (52%)	41,57,57	4.66	18 (43%)
3	GAR	B	623	-	17,18,18	3.59	6 (35%)	21,26,26	1.95	2 (9%)

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	KEU	C	710	-	4/4/11/14	13/41/58/58	0/2/2/2
2	KEU	A	510	-	4/4/11/14	11/41/58/58	0/2/2/2
2	KEU	B	610	-	4/4/11/14	11/41/58/58	0/2/2/2
3	GAR	A	523	-	1/1/6/7	4/12/28/28	0/1/1/1
2	KEU	D	810	-	4/4/11/14	10/41/58/58	0/2/2/2
3	GAR	B	623	-	1/1/6/7	9/12/28/28	0/1/1/1

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	810	KEU	OA2-C5	-22.96	1.17	1.40
2	C	710	KEU	OA2-C5	-22.14	1.17	1.40
2	A	510	KEU	OA2-C5	-20.59	1.19	1.40
2	D	810	KEU	OA1-C5	20.32	1.60	1.40
2	B	610	KEU	OA2-C5	-20.32	1.19	1.40
2	B	610	KEU	OA1-C5	19.98	1.60	1.40
2	A	510	KEU	OA1-C5	19.56	1.59	1.40
2	C	710	KEU	OA1-C5	19.45	1.59	1.40
2	B	610	KEU	C9-N3	18.60	1.62	1.33
2	C	710	KEU	C9-N3	18.52	1.62	1.33
2	D	810	KEU	C9-N3	18.44	1.62	1.33
2	A	510	KEU	C9-N3	18.01	1.61	1.33
2	A	510	KEU	C4-C9	-10.85	1.35	1.51
3	B	623	GAR	O22-C21	10.62	1.44	1.23
2	C	710	KEU	C4-C9	-10.56	1.36	1.51
3	A	523	GAR	O22-C21	10.24	1.44	1.23
2	D	810	KEU	C4-C9	-10.19	1.36	1.51
2	B	610	KEU	C4-C9	-10.07	1.36	1.51
2	C	710	KEU	C12-C11	10.04	1.55	1.39
2	D	810	KEU	C12-C11	9.97	1.55	1.39
2	A	510	KEU	C12-C11	9.71	1.54	1.39
2	B	610	KEU	C12-C11	9.48	1.54	1.39
2	D	810	KEU	O1-C9	8.62	1.40	1.23
2	A	510	KEU	C11-C10	8.44	1.64	1.51
2	B	610	KEU	C11-C10	8.33	1.64	1.51
2	C	710	KEU	O1-C9	8.32	1.39	1.23
2	B	610	KEU	O1-C9	8.06	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	510	KEU	O1-C9	8.06	1.39	1.23
2	C	710	KEU	C11-C10	7.80	1.63	1.51
2	D	810	KEU	C11-C10	7.61	1.63	1.51
2	A	510	KEU	C13-C14	6.77	1.50	1.39
2	C	710	KEU	C13-C14	6.65	1.50	1.39
2	D	810	KEU	C13-C14	6.56	1.50	1.39
2	C	710	KEU	C15-C14	6.28	1.50	1.39
3	A	523	GAR	P15-O16	6.11	1.70	1.50
2	B	610	KEU	C13-C14	6.06	1.49	1.39
2	B	610	KEU	C15-C14	6.04	1.49	1.39
2	D	810	KEU	C15-C14	5.92	1.49	1.39
3	B	623	GAR	P15-O16	5.92	1.69	1.50
2	A	510	KEU	C15-C14	5.45	1.48	1.39
3	A	523	GAR	C21-N19	5.42	1.45	1.34
2	B	610	KEU	C16-C11	5.39	1.47	1.39
2	A	510	KEU	C16-C11	5.39	1.47	1.39
2	C	710	KEU	C16-C11	5.19	1.47	1.39
3	B	623	GAR	C21-N19	5.05	1.44	1.34
2	D	810	KEU	C16-C11	4.92	1.47	1.39
2	C	710	KEU	C2-C1	4.13	1.69	1.52
2	D	810	KEU	C2-C1	4.10	1.69	1.52
3	B	623	GAR	P15-O18	4.04	1.70	1.54
2	B	610	KEU	C2-C1	4.00	1.69	1.52
3	A	523	GAR	P15-O17	3.93	1.70	1.54
3	B	623	GAR	P15-O17	3.82	1.69	1.54
3	A	523	GAR	P15-O18	3.73	1.69	1.54
3	A	523	GAR	C3-N19	3.69	1.47	1.43
2	A	510	KEU	C2-C1	3.65	1.67	1.52
2	A	510	KEU	C12-C13	3.48	1.45	1.38
3	B	623	GAR	C3-N19	3.35	1.47	1.43
2	D	810	KEU	C12-C13	3.23	1.44	1.38
2	B	610	KEU	C12-C13	3.18	1.44	1.38
2	C	710	KEU	C12-C13	3.15	1.44	1.38
2	A	510	KEU	C3-C4	-3.04	1.48	1.54
2	C	710	KEU	C17-N	3.02	1.52	1.45
2	B	610	KEU	C14-C	-2.97	1.44	1.50
2	A	510	KEU	C17-N	2.92	1.52	1.45
2	D	810	KEU	C17-N	2.91	1.52	1.45
2	B	610	KEU	C17-N	2.89	1.52	1.45
2	A	510	KEU	C14-C	-2.78	1.44	1.50
2	C	710	KEU	C17-C18	2.59	1.59	1.52
2	D	810	KEU	C17-C18	2.57	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	710	KEU	C14-C	-2.38	1.45	1.50
2	A	510	KEU	C17-C18	2.23	1.58	1.52
2	D	810	KEU	C-N	2.18	1.38	1.34
2	B	610	KEU	C17-C18	2.15	1.58	1.52
2	D	810	KEU	O2-C18	2.14	1.37	1.30
2	D	810	KEU	C14-C	-2.14	1.45	1.50
2	A	510	KEU	O2-C18	2.11	1.37	1.30
2	D	810	KEU	C3-C4	-2.08	1.50	1.54
2	C	710	KEU	C-N	2.07	1.38	1.34
2	C	710	KEU	O2-C18	2.07	1.37	1.30
2	B	610	KEU	O2-C18	2.05	1.37	1.30

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	610	KEU	O1-C9-N3	-17.76	98.82	122.69
2	D	810	KEU	O1-C9-N3	-17.75	98.83	122.69
2	C	710	KEU	O1-C9-N3	-17.35	99.37	122.69
2	A	510	KEU	O1-C9-N3	-16.90	99.97	122.69
2	D	810	KEU	F1-C6-C5	-13.58	96.84	111.96
2	C	710	KEU	F1-C6-C5	-13.07	97.41	111.96
2	A	510	KEU	C5-C10-C11	11.95	127.66	114.14
2	A	510	KEU	F1-C6-C5	-11.53	99.12	111.96
2	B	610	KEU	F1-C6-C5	-9.39	101.51	111.96
2	A	510	KEU	C2-C3-C4	-8.53	98.96	114.28
2	B	610	KEU	C5-C10-C11	8.41	123.66	114.14
2	C	710	KEU	C2-C3-C4	-8.07	99.78	114.28
2	D	810	KEU	C2-C3-C4	-8.00	99.90	114.28
2	A	510	KEU	C16-C11-C10	-7.87	105.31	121.08
2	B	610	KEU	C2-C3-C4	-7.71	100.43	114.28
2	D	810	KEU	O1-C9-C4	7.58	135.04	122.04
2	C	710	KEU	C5-C10-C11	7.54	122.67	114.14
3	A	523	GAR	O22-C21-N19	-7.52	110.26	122.95
3	B	623	GAR	O22-C21-N19	-7.49	110.30	122.95
2	D	810	KEU	C5-C10-C11	7.22	122.30	114.14
2	B	610	KEU	O1-C9-C4	7.21	134.40	122.04
2	A	510	KEU	O1-C9-C4	7.09	134.20	122.04
2	C	710	KEU	O1-C9-C4	6.88	133.84	122.04
2	D	810	KEU	F2-C6-C5	6.09	118.74	111.96
2	B	610	KEU	F2-C6-C5	5.93	118.56	111.96
2	A	510	KEU	C12-C11-C10	5.92	132.92	121.08
2	C	710	KEU	F2-C6-C5	5.70	118.31	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	510	KEU	OA2-C5-C6	5.69	122.25	107.41
2	B	610	KEU	C2-C1-C10	-5.38	101.11	113.68
2	C	710	KEU	C2-C1-C10	-5.21	101.50	113.68
2	B	610	KEU	OA1-C5-C6	-5.20	93.84	107.41
2	B	610	KEU	OA2-C5-C6	4.93	120.28	107.41
2	D	810	KEU	C16-C11-C10	-4.89	111.28	121.08
2	C	710	KEU	OA2-C5-C6	4.81	119.96	107.41
2	C	710	KEU	C16-C11-C10	-4.81	111.44	121.08
2	B	610	KEU	C16-C11-C10	-4.77	111.52	121.08
2	D	810	KEU	C2-C1-C10	-4.72	102.65	113.68
2	D	810	KEU	OA2-C5-C6	4.55	119.29	107.41
2	C	710	KEU	OA1-C5-C6	-4.43	95.86	107.41
2	A	510	KEU	C13-C12-C11	-4.36	116.81	121.20
2	C	710	KEU	C13-C12-C11	-4.20	116.97	121.20
2	D	810	KEU	C13-C12-C11	-4.14	117.03	121.20
2	B	610	KEU	C4-C9-N3	4.09	126.76	116.65
2	C	710	KEU	C4-C9-N3	4.00	126.55	116.65
2	D	810	KEU	OA1-C5-C6	-3.98	97.03	107.41
2	A	510	KEU	F2-C6-C5	3.86	116.26	111.96
2	D	810	KEU	C4-C9-N3	3.74	125.91	116.65
2	B	610	KEU	C13-C12-C11	-3.74	117.44	121.20
2	A	510	KEU	C4-C9-N3	3.67	125.74	116.65
2	A	510	KEU	OA1-C5-C6	-3.60	98.01	107.41
2	C	710	KEU	OA1-C5-OA2	-3.56	100.55	110.89
2	C	710	KEU	C19-C17-N	-3.39	104.01	110.88
2	D	810	KEU	C12-C11-C10	3.37	127.83	121.08
2	D	810	KEU	OA1-C5-OA2	-3.34	101.20	110.89
2	A	510	KEU	C15-C14-C13	3.16	123.09	118.59
2	C	710	KEU	C12-C11-C10	3.10	127.29	121.08
2	B	610	KEU	C15-C14-C13	3.09	122.98	118.59
2	B	610	KEU	C12-C11-C10	3.06	127.21	121.08
2	B	610	KEU	C19-C17-N	-2.95	104.91	110.88
2	B	610	KEU	OA1-C5-OA2	-2.87	102.56	110.89
2	A	510	KEU	C16-C15-C14	-2.65	117.69	120.78
2	C	710	KEU	C19-C17-C18	2.58	116.56	110.35
3	A	523	GAR	C1-C2-C3	2.57	106.30	101.42
2	A	510	KEU	C19-C17-N	-2.55	105.72	110.88
2	A	510	KEU	C19-C17-C18	2.53	116.44	110.35
2	A	510	KEU	O2-C18-C17	2.49	121.68	113.40
2	D	810	KEU	C19-C17-N	-2.47	105.88	110.88
2	B	610	KEU	O2-C18-C17	2.46	121.58	113.40
3	B	623	GAR	O12-C10-C5	2.44	117.38	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	610	KEU	C16-C15-C14	-2.34	118.06	120.78
2	A	510	KEU	C16-C11-C12	2.32	121.19	118.29
2	B	610	KEU	C16-C11-C12	2.31	121.17	118.29
2	C	710	KEU	C16-C11-C12	2.27	121.12	118.29
2	D	810	KEU	O2-C18-C17	2.24	120.85	113.40
2	C	710	KEU	C15-C14-C13	2.20	121.72	118.59
2	C	710	KEU	O2-C18-C17	2.11	120.41	113.40
2	B	610	KEU	F-C6-C5	-2.09	109.63	111.96
2	D	810	KEU	C19-C17-C18	2.07	115.34	110.35
3	A	523	GAR	C5-O4-C3	2.02	112.83	108.49
2	D	810	KEU	C16-C11-C12	2.00	120.79	118.29

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	510	KEU	C7
2	A	510	KEU	C10
2	A	510	KEU	C4
2	A	510	KEU	C8
2	B	610	KEU	C7
2	B	610	KEU	C10
2	B	610	KEU	C4
2	B	610	KEU	C8
2	C	710	KEU	C7
2	C	710	KEU	C10
2	C	710	KEU	C4
2	C	710	KEU	C8
2	D	810	KEU	C7
2	D	810	KEU	C10
2	D	810	KEU	C4
2	D	810	KEU	C8
3	A	523	GAR	C1
3	B	623	GAR	C1

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	510	KEU	C11-C10-C5-OA2
2	A	510	KEU	C11-C10-C5-OA1
2	A	510	KEU	C11-C10-C5-C6
2	A	510	KEU	C1-C10-C5-OA1
2	A	510	KEU	C2-C3-C4-C9

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Mol	Chain	Res	Type	Atoms
2	A	510	KEU	OA2-C5-C6-F1
2	A	510	KEU	OA2-C5-C6-F
2	B	610	KEU	C11-C10-C5-OA2
2	B	610	KEU	C11-C10-C5-OA1
2	B	610	KEU	C1-C10-C5-OA2
2	B	610	KEU	C1-C10-C5-OA1
2	B	610	KEU	C2-C3-C4-C9
2	B	610	KEU	OA2-C5-C6-F1
2	B	610	KEU	OA2-C5-C6-F
2	C	710	KEU	C11-C10-C5-OA2
2	C	710	KEU	C11-C10-C5-OA1
2	C	710	KEU	C1-C10-C5-OA2
2	C	710	KEU	C1-C10-C5-OA1
2	C	710	KEU	C2-C3-C4-C9
2	C	710	KEU	OA2-C5-C6-F2
2	C	710	KEU	OA2-C5-C6-F1
2	C	710	KEU	OA2-C5-C6-F
2	D	810	KEU	C11-C10-C5-OA2
2	D	810	KEU	C11-C10-C5-OA1
2	D	810	KEU	C1-C10-C5-OA2
2	D	810	KEU	C1-C10-C5-OA1
2	D	810	KEU	C2-C3-C4-C9
2	D	810	KEU	OA2-C5-C6-F1
2	D	810	KEU	OA2-C5-C6-F
3	A	523	GAR	O4-C3-N19-C21
3	A	523	GAR	O22-C21-N19-C3
3	B	623	GAR	O4-C3-N19-C21
3	B	623	GAR	C10-O12-P15-O17
3	B	623	GAR	C10-O12-P15-O18
3	B	623	GAR	O22-C21-N19-C3
2	A	510	KEU	C2-C1-C10-C11
3	B	623	GAR	O12-C10-C5-C1
3	B	623	GAR	O12-C10-C5-O4
3	B	623	GAR	C23-C21-N19-C3
2	B	610	KEU	C1-C2-C3-C4
2	C	710	KEU	C1-C2-C3-C4
2	D	810	KEU	C1-C2-C3-C4
2	A	510	KEU	C1-C10-C11-C16
2	B	610	KEU	C2-C1-C10-C11
2	C	710	KEU	C10-C1-C2-C3
2	D	810	KEU	C10-C1-C2-C3
3	A	523	GAR	O22-C21-C23-N24

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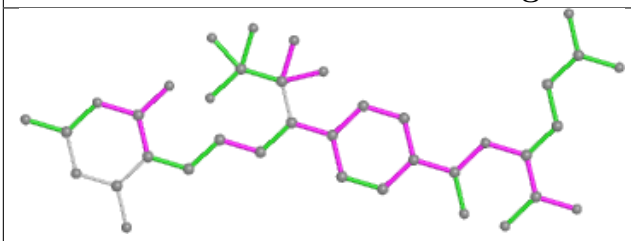
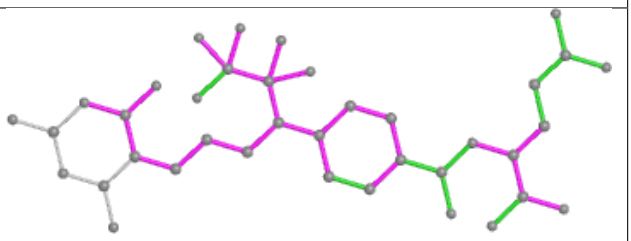
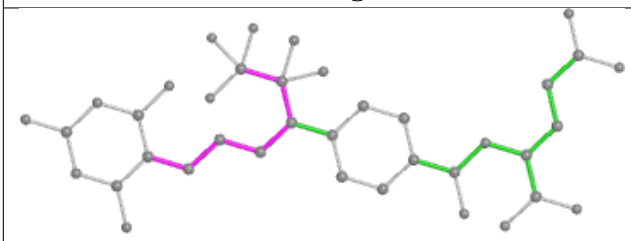
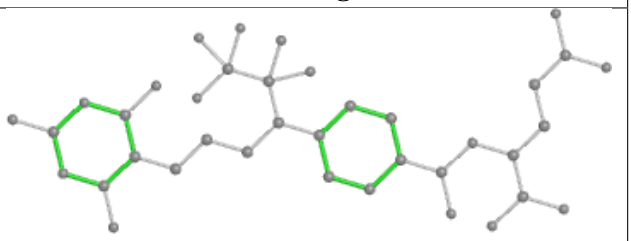
Mol	Chain	Res	Type	Atoms
3	B	623	GAR	O22-C21-C23-N24
2	C	710	KEU	C2-C1-C10-C11
2	A	510	KEU	C2-C1-C10-C5
2	B	610	KEU	C2-C1-C10-C5
2	C	710	KEU	C2-C1-C10-C5
2	D	810	KEU	C2-C1-C10-C5
2	B	610	KEU	C10-C1-C2-C3
2	A	510	KEU	C5-C10-C11-C12
2	C	710	KEU	OA1-C5-C6-F
3	B	623	GAR	C10-O12-P15-O16
3	A	523	GAR	O12-C10-C5-O4

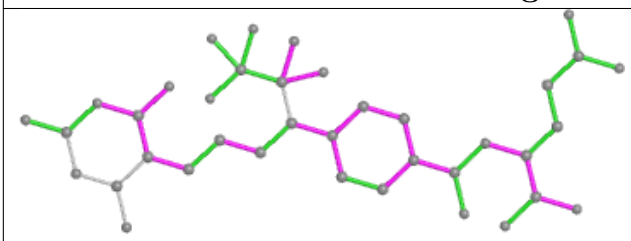
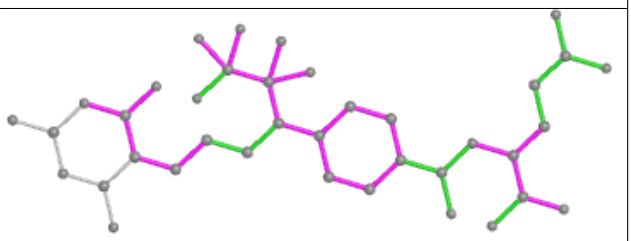
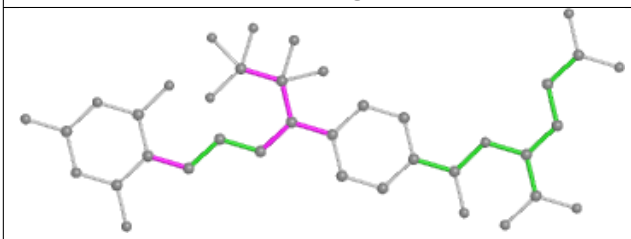
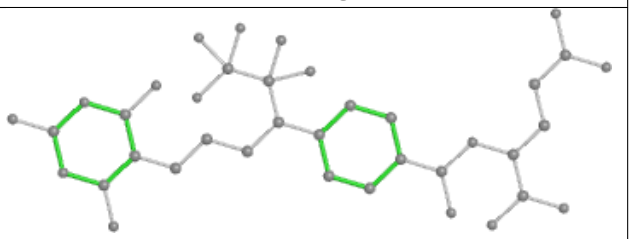
There are no ring outliers.

6 monomers are involved in 27 short contacts:

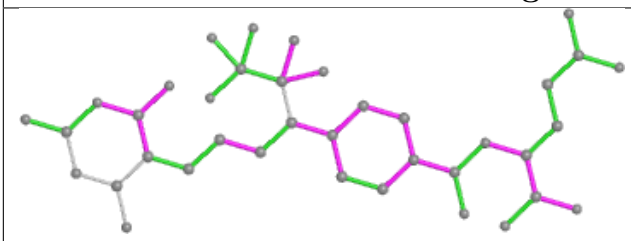
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	710	KEU	3	0
2	A	510	KEU	2	0
2	B	610	KEU	4	0
3	A	523	GAR	7	0
2	D	810	KEU	2	0
3	B	623	GAR	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

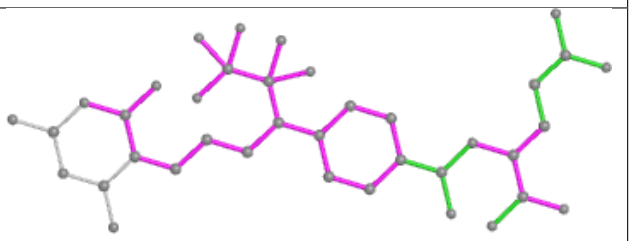
Ligand KEU C 710	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KEU A 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

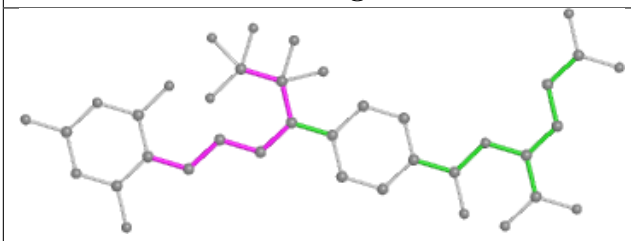
Ligand KEU B 610



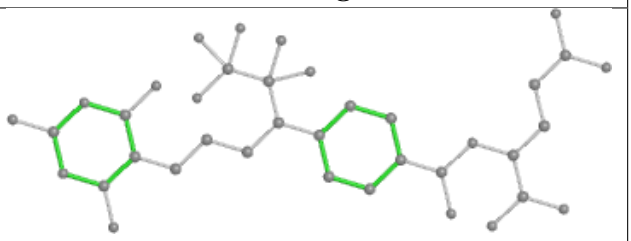
Bond lengths



Bond angles

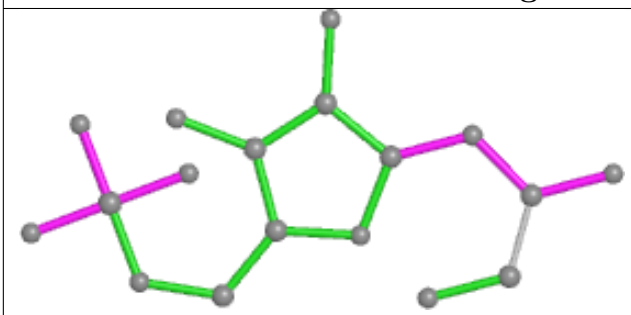


Torsions

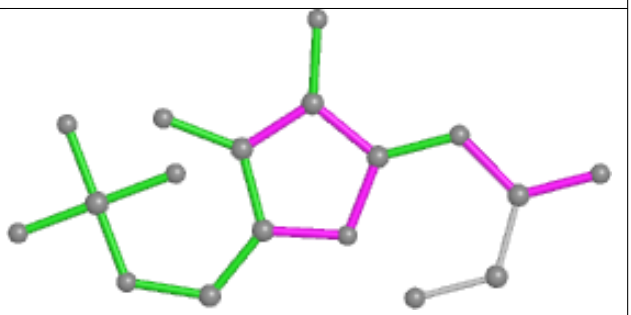


Rings

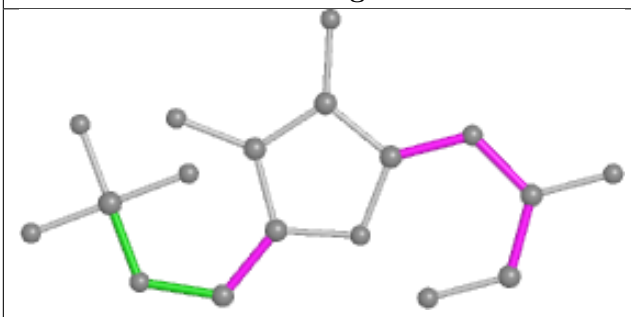
Ligand GAR A 523



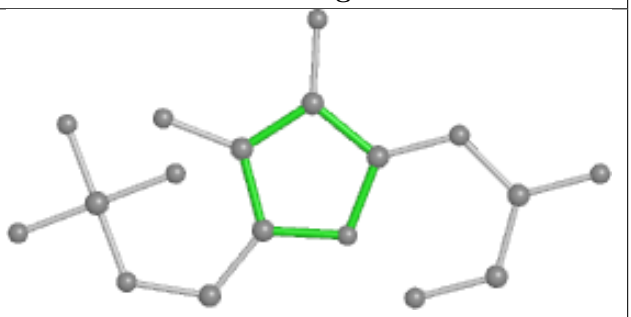
Bond lengths



Bond angles

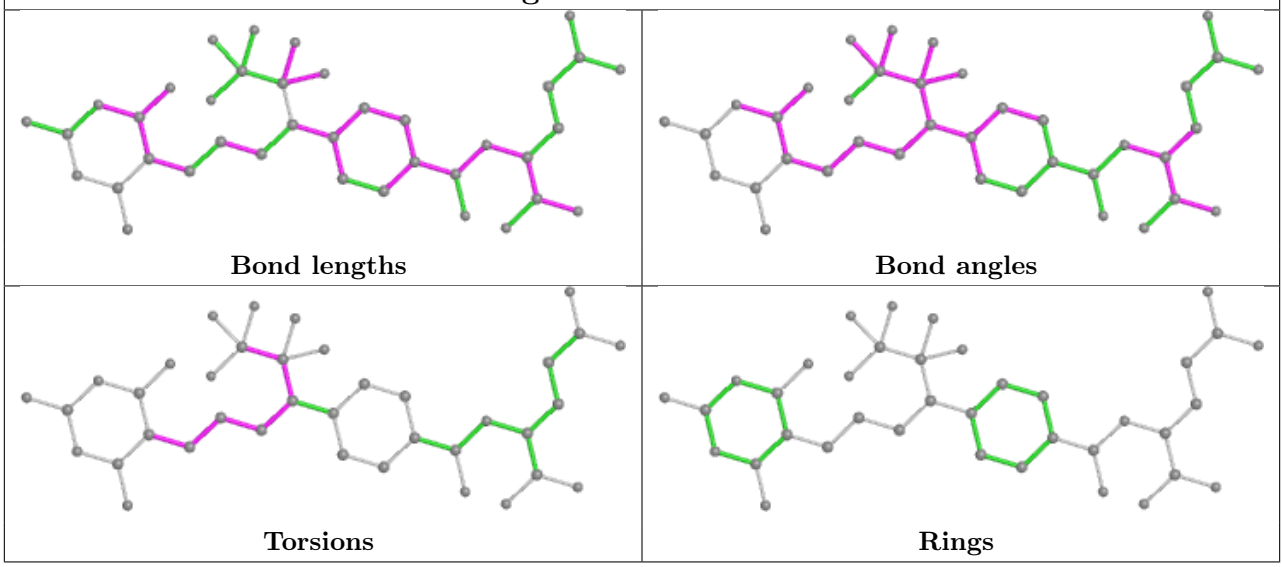


Torsions

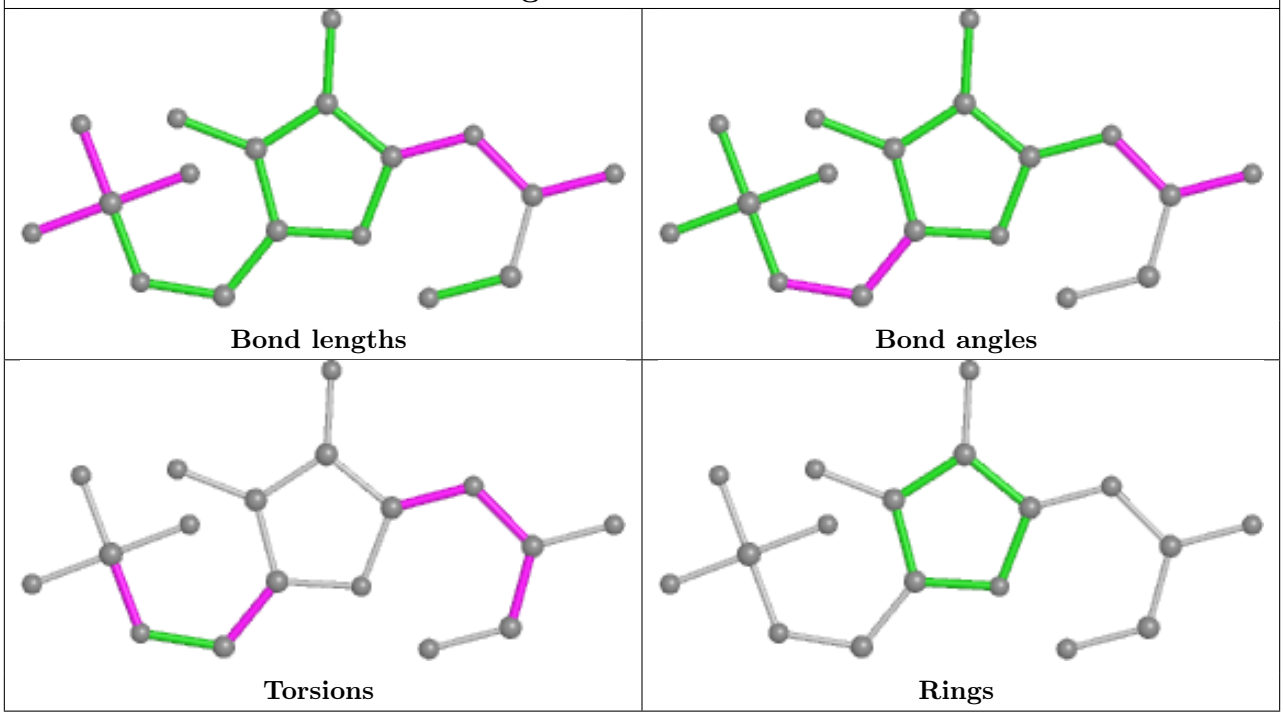


Rings

Ligand KEU D 810



Ligand GAR B 623



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	200/209 (95%)	-0.10	3 (1%)	73	77	19, 29, 45, 63	0
1	B	200/209 (95%)	-0.06	1 (0%)	91	92	18, 29, 46, 63	0
1	C	200/209 (95%)	0.06	4 (2%)	65	69	19, 33, 57, 72	0
1	D	200/209 (95%)	0.07	3 (1%)	73	77	19, 32, 55, 71	0
All	All	800/836 (95%)	-0.01	11 (1%)	75	78	18, 31, 52, 72	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	VAL	4.3
1	A	196	LYS	3.7
1	D	193	GLU	3.4
1	A	192	GLY	3.0
1	C	62	LYS	2.9
1	D	24	PRO	2.7
1	C	73	LEU	2.7
1	C	197	ILE	2.4
1	D	98	GLN	2.3
1	B	60	LEU	2.2
1	A	200	VAL	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

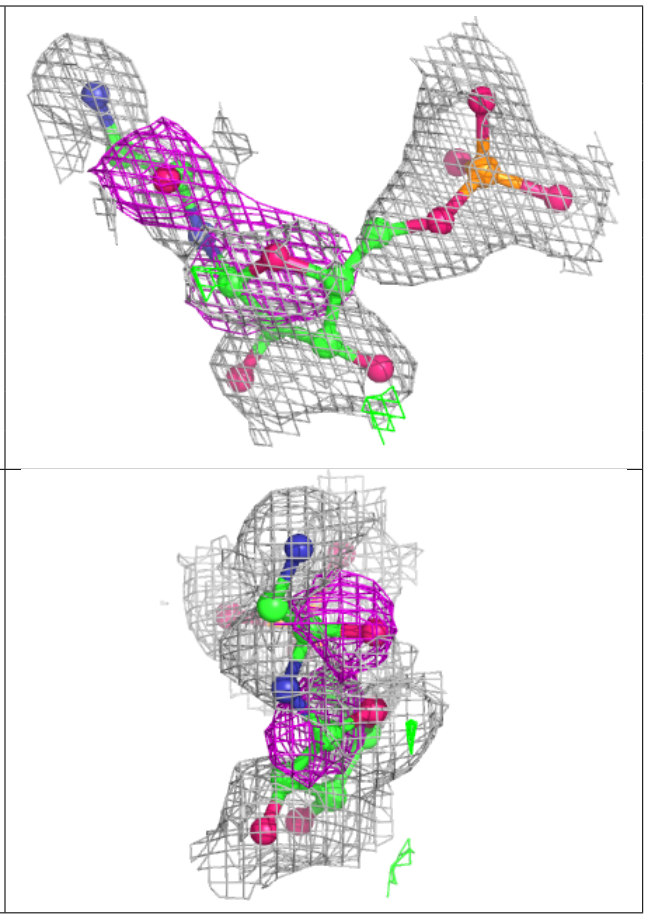
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

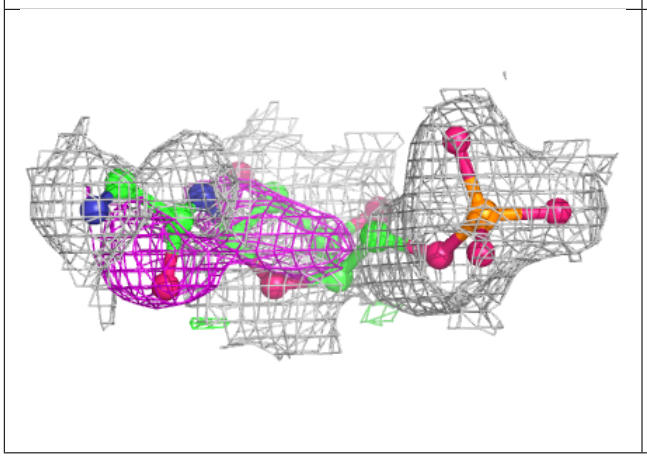
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GAR	B	623	18/18	0.78	0.26	33,44,48,49	0
2	KEU	D	810	38/38	0.87	0.14	28,33,49,52	0
2	KEU	C	710	38/38	0.89	0.14	30,35,48,51	0
3	GAR	A	523	18/18	0.90	0.22	36,48,52,53	0
2	KEU	A	510	38/38	0.93	0.11	20,24,29,30	0
2	KEU	B	610	38/38	0.94	0.12	20,25,29,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GAR B 623:

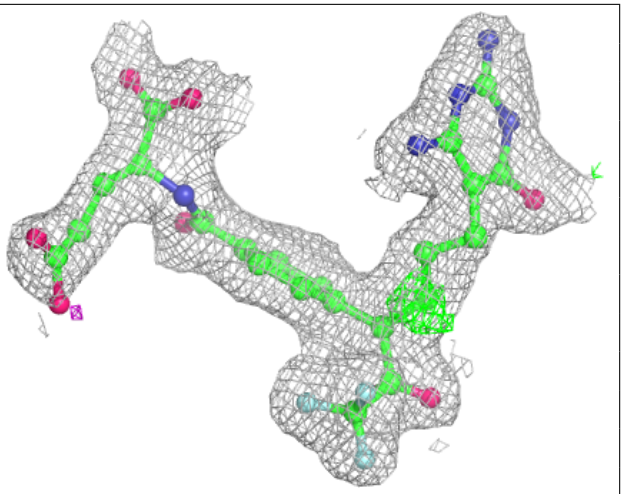
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

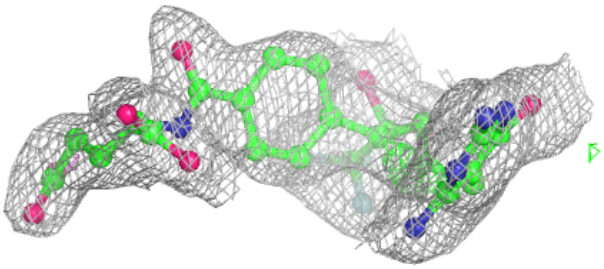


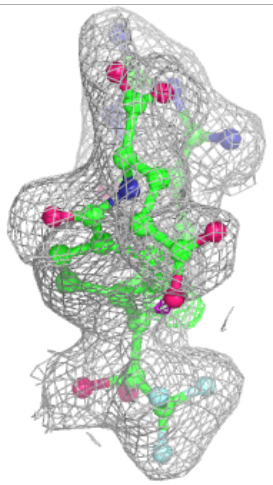


Electron density around KEU D 810:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

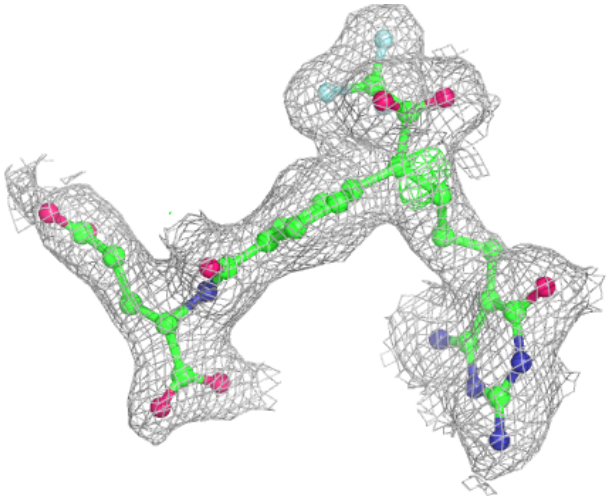


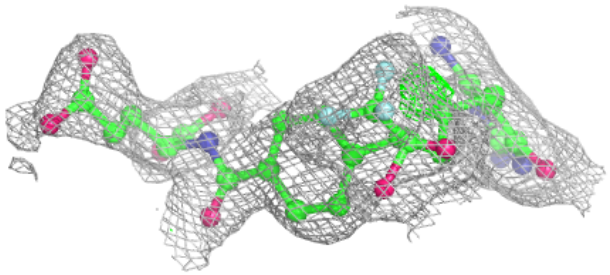


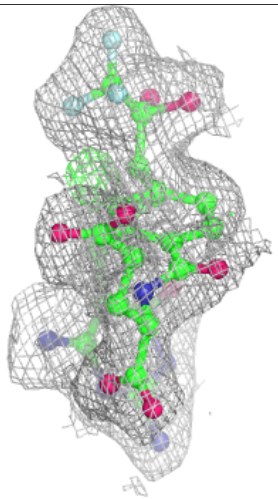


Electron density around KEU C 710:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

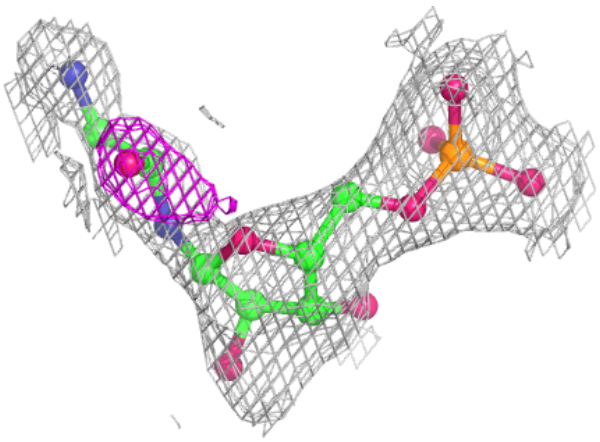


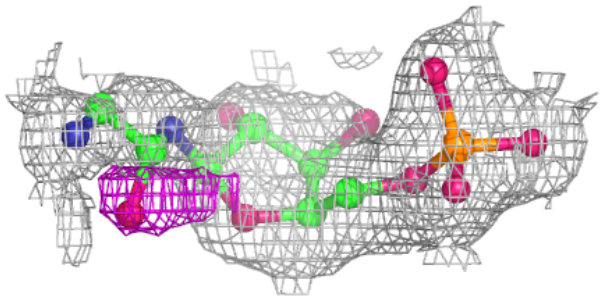


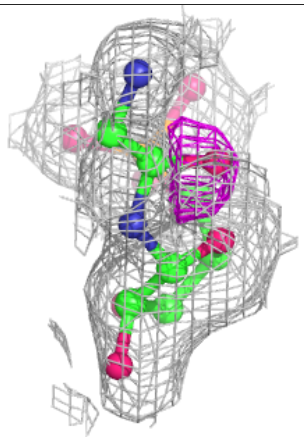


Electron density around GAR A 523:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

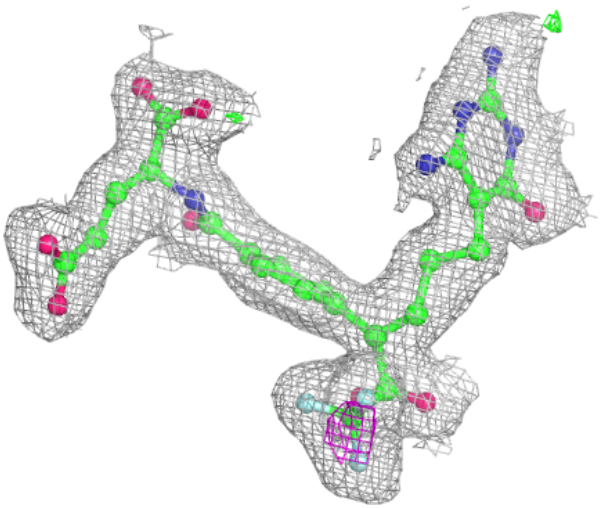


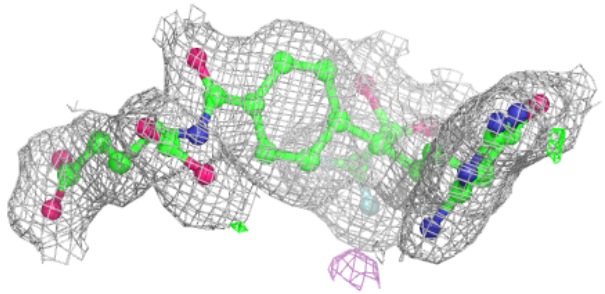


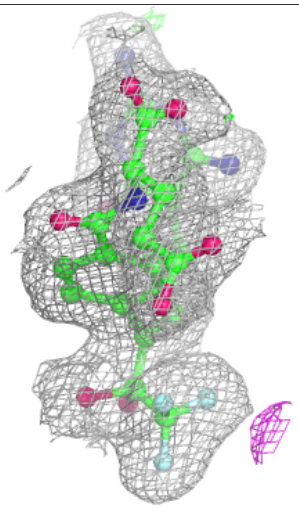


Electron density around KEU A 510:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

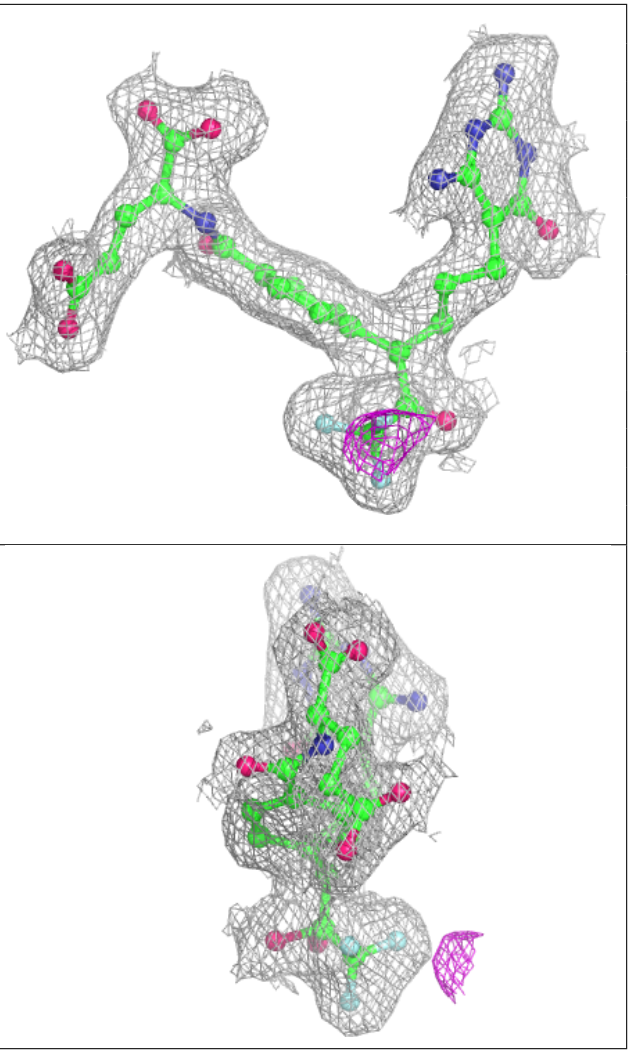






Electron density around KEU B 610:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.