wwPDB X-ray Structure Validation Summary Report (i)

Jul 12, 2022 – 01:12 pm BST

PDB ID	:	7QG6
Title	:	Co-crystal structure of UPF3A-RRM-NOPS-L with UPF2-MIF4GIII
Authors	:	Powers, K.T.; Bufton, J.C.; Szeto, J.A.; Schaffitzel, C.
Deposited on	:	2021-12-07
Resolution	:	2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

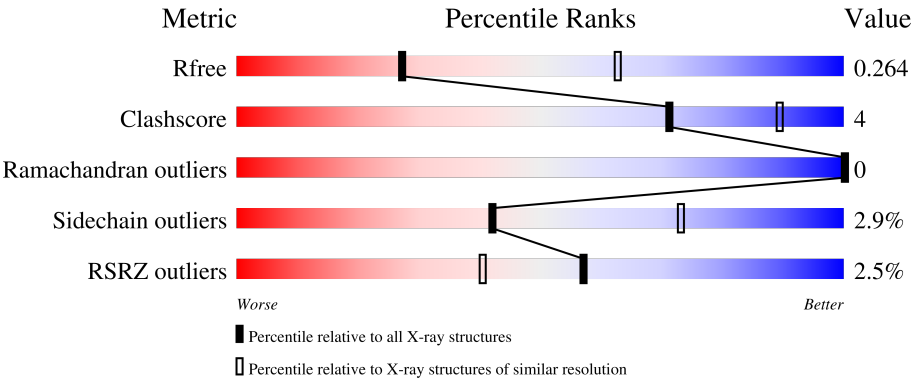
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	176	2% 60% 10% 30%
1	C	176	63% • 34%
1	E	176	5% 57% 11% 32%
1	G	176	3% 61% 5% • 34%
2	B	321	% 68% 10% 23%

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Mol	Chain	Length	Quality of chain
2	D	321	64% 11% 24%
2	F	321	% 71% 6% 23%
2	H	321	3% 70% 6% 24%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11757 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 Regulator of nonsense transcripts 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	117	Total	C	N	O	S	0	0	0
			928	610	148	169	1			
1	A	123	Total	C	N	O	S	0	0	0
			965	632	154	178	1			
1	E	119	Total	C	N	O	S	0	0	0
			904	593	142	168	1			
1	G	116	Total	C	N	O	S	0	0	0
			901	595	140	165	1			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	31	MET	-	initiating methionine	UNP Q9H1J1
C	32	SER	-	expression tag	UNP Q9H1J1
C	33	TYR	-	expression tag	UNP Q9H1J1
C	34	TYR	-	expression tag	UNP Q9H1J1
C	35	HIS	-	expression tag	UNP Q9H1J1
C	36	HIS	-	expression tag	UNP Q9H1J1
C	37	HIS	-	expression tag	UNP Q9H1J1
C	38	HIS	-	expression tag	UNP Q9H1J1
C	39	HIS	-	expression tag	UNP Q9H1J1
C	40	HIS	-	expression tag	UNP Q9H1J1
C	41	ASP	-	expression tag	UNP Q9H1J1
C	42	TYR	-	expression tag	UNP Q9H1J1
C	43	ASP	-	expression tag	UNP Q9H1J1
C	44	ILE	-	expression tag	UNP Q9H1J1
C	45	PRO	-	expression tag	UNP Q9H1J1
C	46	THR	-	expression tag	UNP Q9H1J1
C	47	THR	-	expression tag	UNP Q9H1J1
C	48	GLU	-	expression tag	UNP Q9H1J1
C	49	ASN	-	expression tag	UNP Q9H1J1
C	50	LEU	-	expression tag	UNP Q9H1J1
C	51	TYR	-	expression tag	UNP Q9H1J1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	52	PHE	-	expression tag	UNP Q9H1J1
C	53	GLN	-	expression tag	UNP Q9H1J1
C	54	GLY	-	expression tag	UNP Q9H1J1
C	55	ALA	-	expression tag	UNP Q9H1J1
C	56	MET	-	expression tag	UNP Q9H1J1
C	57	ASP	-	expression tag	UNP Q9H1J1
A	31	MET	-	initiating methionine	UNP Q9H1J1
A	32	SER	-	expression tag	UNP Q9H1J1
A	33	TYR	-	expression tag	UNP Q9H1J1
A	34	TYR	-	expression tag	UNP Q9H1J1
A	35	HIS	-	expression tag	UNP Q9H1J1
A	36	HIS	-	expression tag	UNP Q9H1J1
A	37	HIS	-	expression tag	UNP Q9H1J1
A	38	HIS	-	expression tag	UNP Q9H1J1
A	39	HIS	-	expression tag	UNP Q9H1J1
A	40	HIS	-	expression tag	UNP Q9H1J1
A	41	ASP	-	expression tag	UNP Q9H1J1
A	42	TYR	-	expression tag	UNP Q9H1J1
A	43	ASP	-	expression tag	UNP Q9H1J1
A	44	ILE	-	expression tag	UNP Q9H1J1
A	45	PRO	-	expression tag	UNP Q9H1J1
A	46	THR	-	expression tag	UNP Q9H1J1
A	47	THR	-	expression tag	UNP Q9H1J1
A	48	GLU	-	expression tag	UNP Q9H1J1
A	49	ASN	-	expression tag	UNP Q9H1J1
A	50	LEU	-	expression tag	UNP Q9H1J1
A	51	TYR	-	expression tag	UNP Q9H1J1
A	52	PHE	-	expression tag	UNP Q9H1J1
A	53	GLN	-	expression tag	UNP Q9H1J1
A	54	GLY	-	expression tag	UNP Q9H1J1
A	55	ALA	-	expression tag	UNP Q9H1J1
A	56	MET	-	expression tag	UNP Q9H1J1
A	57	ASP	-	expression tag	UNP Q9H1J1
E	31	MET	-	initiating methionine	UNP Q9H1J1
E	32	SER	-	expression tag	UNP Q9H1J1
E	33	TYR	-	expression tag	UNP Q9H1J1
E	34	TYR	-	expression tag	UNP Q9H1J1
E	35	HIS	-	expression tag	UNP Q9H1J1
E	36	HIS	-	expression tag	UNP Q9H1J1
E	37	HIS	-	expression tag	UNP Q9H1J1
E	38	HIS	-	expression tag	UNP Q9H1J1
E	39	HIS	-	expression tag	UNP Q9H1J1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	40	HIS	-	expression tag	UNP Q9H1J1
E	41	ASP	-	expression tag	UNP Q9H1J1
E	42	TYR	-	expression tag	UNP Q9H1J1
E	43	ASP	-	expression tag	UNP Q9H1J1
E	44	ILE	-	expression tag	UNP Q9H1J1
E	45	PRO	-	expression tag	UNP Q9H1J1
E	46	THR	-	expression tag	UNP Q9H1J1
E	47	THR	-	expression tag	UNP Q9H1J1
E	48	GLU	-	expression tag	UNP Q9H1J1
E	49	ASN	-	expression tag	UNP Q9H1J1
E	50	LEU	-	expression tag	UNP Q9H1J1
E	51	TYR	-	expression tag	UNP Q9H1J1
E	52	PHE	-	expression tag	UNP Q9H1J1
E	53	GLN	-	expression tag	UNP Q9H1J1
E	54	GLY	-	expression tag	UNP Q9H1J1
E	55	ALA	-	expression tag	UNP Q9H1J1
E	56	MET	-	expression tag	UNP Q9H1J1
E	57	ASP	-	expression tag	UNP Q9H1J1
G	31	MET	-	initiating methionine	UNP Q9H1J1
G	32	SER	-	expression tag	UNP Q9H1J1
G	33	TYR	-	expression tag	UNP Q9H1J1
G	34	TYR	-	expression tag	UNP Q9H1J1
G	35	HIS	-	expression tag	UNP Q9H1J1
G	36	HIS	-	expression tag	UNP Q9H1J1
G	37	HIS	-	expression tag	UNP Q9H1J1
G	38	HIS	-	expression tag	UNP Q9H1J1
G	39	HIS	-	expression tag	UNP Q9H1J1
G	40	HIS	-	expression tag	UNP Q9H1J1
G	41	ASP	-	expression tag	UNP Q9H1J1
G	42	TYR	-	expression tag	UNP Q9H1J1
G	43	ASP	-	expression tag	UNP Q9H1J1
G	44	ILE	-	expression tag	UNP Q9H1J1
G	45	PRO	-	expression tag	UNP Q9H1J1
G	46	THR	-	expression tag	UNP Q9H1J1
G	47	THR	-	expression tag	UNP Q9H1J1
G	48	GLU	-	expression tag	UNP Q9H1J1
G	49	ASN	-	expression tag	UNP Q9H1J1
G	50	LEU	-	expression tag	UNP Q9H1J1
G	51	TYR	-	expression tag	UNP Q9H1J1
G	52	PHE	-	expression tag	UNP Q9H1J1
G	53	GLN	-	expression tag	UNP Q9H1J1
G	54	GLY	-	expression tag	UNP Q9H1J1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	55	ALA	-	expression tag	UNP Q9H1J1
G	56	MET	-	expression tag	UNP Q9H1J1
G	57	ASP	-	expression tag	UNP Q9H1J1

- Molecule 2 is a protein called Regulator of nonsense transcripts 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	245	Total	C	N	O	S	0	1	0
			2015	1297	343	363	12			
2	B	248	Total	C	N	O	S	0	1	0
			2033	1312	346	363	12			
2	F	246	Total	C	N	O	S	0	0	0
			1987	1282	337	356	12			
2	H	244	Total	C	N	O	S	0	0	0
			1974	1279	335	348	12			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	734	MET	-	initiating methionine	UNP Q9HAU5
D	735	SER	-	expression tag	UNP Q9HAU5
D	736	TYR	-	expression tag	UNP Q9HAU5
D	737	TYR	-	expression tag	UNP Q9HAU5
D	738	HIS	-	expression tag	UNP Q9HAU5
D	739	HIS	-	expression tag	UNP Q9HAU5
D	740	HIS	-	expression tag	UNP Q9HAU5
D	741	HIS	-	expression tag	UNP Q9HAU5
D	742	HIS	-	expression tag	UNP Q9HAU5
D	743	HIS	-	expression tag	UNP Q9HAU5
D	744	ASP	-	expression tag	UNP Q9HAU5
D	745	TYR	-	expression tag	UNP Q9HAU5
D	746	ASP	-	expression tag	UNP Q9HAU5
D	747	ILE	-	expression tag	UNP Q9HAU5
D	748	PRO	-	expression tag	UNP Q9HAU5
D	749	THR	-	expression tag	UNP Q9HAU5
D	750	THR	-	expression tag	UNP Q9HAU5
D	751	GLU	-	expression tag	UNP Q9HAU5
D	752	ASN	-	expression tag	UNP Q9HAU5
D	753	LEU	-	expression tag	UNP Q9HAU5
D	754	TYR	-	expression tag	UNP Q9HAU5
D	755	PHE	-	expression tag	UNP Q9HAU5
D	756	GLN	-	expression tag	UNP Q9HAU5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	757	GLY	-	expression tag	UNP Q9HAU5
D	758	ALA	-	expression tag	UNP Q9HAU5
D	759	MET	-	expression tag	UNP Q9HAU5
D	760	ASP	-	expression tag	UNP Q9HAU5
B	734	MET	-	initiating methionine	UNP Q9HAU5
B	735	SER	-	expression tag	UNP Q9HAU5
B	736	TYR	-	expression tag	UNP Q9HAU5
B	737	TYR	-	expression tag	UNP Q9HAU5
B	738	HIS	-	expression tag	UNP Q9HAU5
B	739	HIS	-	expression tag	UNP Q9HAU5
B	740	HIS	-	expression tag	UNP Q9HAU5
B	741	HIS	-	expression tag	UNP Q9HAU5
B	742	HIS	-	expression tag	UNP Q9HAU5
B	743	HIS	-	expression tag	UNP Q9HAU5
B	744	ASP	-	expression tag	UNP Q9HAU5
B	745	TYR	-	expression tag	UNP Q9HAU5
B	746	ASP	-	expression tag	UNP Q9HAU5
B	747	ILE	-	expression tag	UNP Q9HAU5
B	748	PRO	-	expression tag	UNP Q9HAU5
B	749	THR	-	expression tag	UNP Q9HAU5
B	750	THR	-	expression tag	UNP Q9HAU5
B	751	GLU	-	expression tag	UNP Q9HAU5
B	752	ASN	-	expression tag	UNP Q9HAU5
B	753	LEU	-	expression tag	UNP Q9HAU5
B	754	TYR	-	expression tag	UNP Q9HAU5
B	755	PHE	-	expression tag	UNP Q9HAU5
B	756	GLN	-	expression tag	UNP Q9HAU5
B	757	GLY	-	expression tag	UNP Q9HAU5
B	758	ALA	-	expression tag	UNP Q9HAU5
B	759	MET	-	expression tag	UNP Q9HAU5
B	760	ASP	-	expression tag	UNP Q9HAU5
F	734	MET	-	initiating methionine	UNP Q9HAU5
F	735	SER	-	expression tag	UNP Q9HAU5
F	736	TYR	-	expression tag	UNP Q9HAU5
F	737	TYR	-	expression tag	UNP Q9HAU5
F	738	HIS	-	expression tag	UNP Q9HAU5
F	739	HIS	-	expression tag	UNP Q9HAU5
F	740	HIS	-	expression tag	UNP Q9HAU5
F	741	HIS	-	expression tag	UNP Q9HAU5
F	742	HIS	-	expression tag	UNP Q9HAU5
F	743	HIS	-	expression tag	UNP Q9HAU5
F	744	ASP	-	expression tag	UNP Q9HAU5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	745	TYR	-	expression tag	UNP Q9HAU5
F	746	ASP	-	expression tag	UNP Q9HAU5
F	747	ILE	-	expression tag	UNP Q9HAU5
F	748	PRO	-	expression tag	UNP Q9HAU5
F	749	THR	-	expression tag	UNP Q9HAU5
F	750	THR	-	expression tag	UNP Q9HAU5
F	751	GLU	-	expression tag	UNP Q9HAU5
F	752	ASN	-	expression tag	UNP Q9HAU5
F	753	LEU	-	expression tag	UNP Q9HAU5
F	754	TYR	-	expression tag	UNP Q9HAU5
F	755	PHE	-	expression tag	UNP Q9HAU5
F	756	GLN	-	expression tag	UNP Q9HAU5
F	757	GLY	-	expression tag	UNP Q9HAU5
F	758	ALA	-	expression tag	UNP Q9HAU5
F	759	MET	-	expression tag	UNP Q9HAU5
F	760	ASP	-	expression tag	UNP Q9HAU5
H	734	MET	-	initiating methionine	UNP Q9HAU5
H	735	SER	-	expression tag	UNP Q9HAU5
H	736	TYR	-	expression tag	UNP Q9HAU5
H	737	TYR	-	expression tag	UNP Q9HAU5
H	738	HIS	-	expression tag	UNP Q9HAU5
H	739	HIS	-	expression tag	UNP Q9HAU5
H	740	HIS	-	expression tag	UNP Q9HAU5
H	741	HIS	-	expression tag	UNP Q9HAU5
H	742	HIS	-	expression tag	UNP Q9HAU5
H	743	HIS	-	expression tag	UNP Q9HAU5
H	744	ASP	-	expression tag	UNP Q9HAU5
H	745	TYR	-	expression tag	UNP Q9HAU5
H	746	ASP	-	expression tag	UNP Q9HAU5
H	747	ILE	-	expression tag	UNP Q9HAU5
H	748	PRO	-	expression tag	UNP Q9HAU5
H	749	THR	-	expression tag	UNP Q9HAU5
H	750	THR	-	expression tag	UNP Q9HAU5
H	751	GLU	-	expression tag	UNP Q9HAU5
H	752	ASN	-	expression tag	UNP Q9HAU5
H	753	LEU	-	expression tag	UNP Q9HAU5
H	754	TYR	-	expression tag	UNP Q9HAU5
H	755	PHE	-	expression tag	UNP Q9HAU5
H	756	GLN	-	expression tag	UNP Q9HAU5
H	757	GLY	-	expression tag	UNP Q9HAU5
H	758	ALA	-	expression tag	UNP Q9HAU5
H	759	MET	-	expression tag	UNP Q9HAU5

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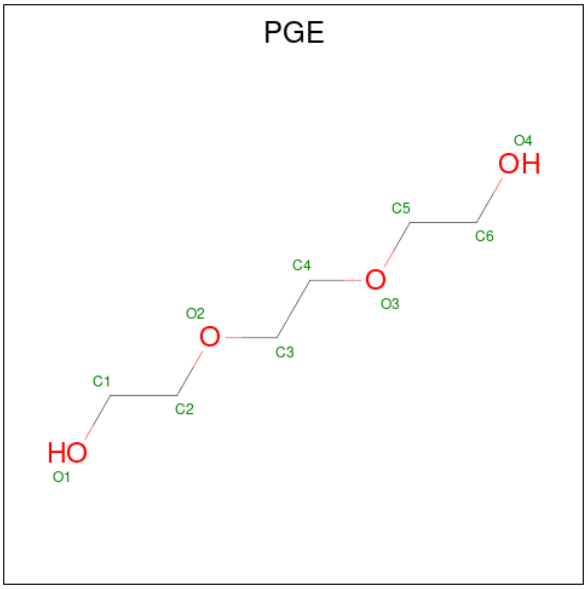
Chain	Residue	Modelled	Actual	Comment	Reference
H	760	ASP	-	expression tag	UNP Q9HAU5

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 10 6 4	0	0
3	B	1	Total C O 10 6 4	0	0
3	F	1	Total C O 10 6 4	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 1 1	0	0
5	D	9	Total O 9 9	0	0

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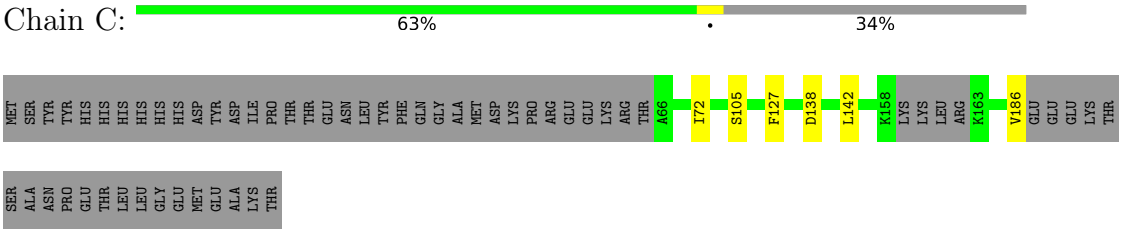
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	2	Total O 2 2	0	0
5	F	1	Total O 1 1	0	0
5	G	2	Total O 2 2	0	0
5	H	3	Total O 3 3	0	0

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.

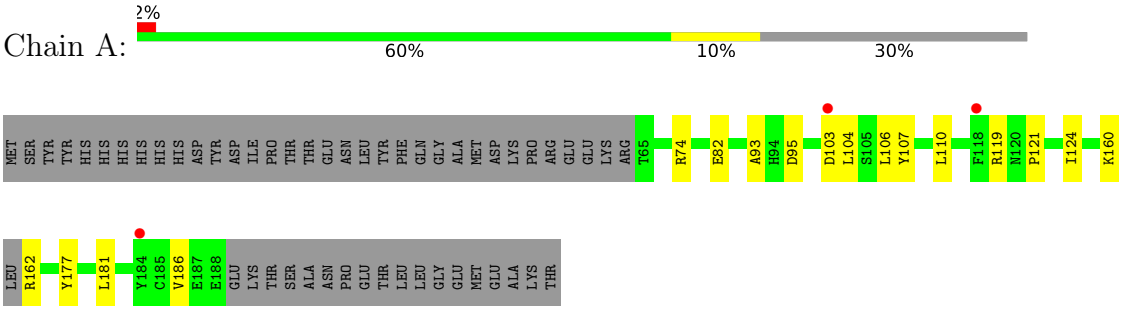
• Molecule 1: Regulator of nonsense transcripts 3A

Chain C:



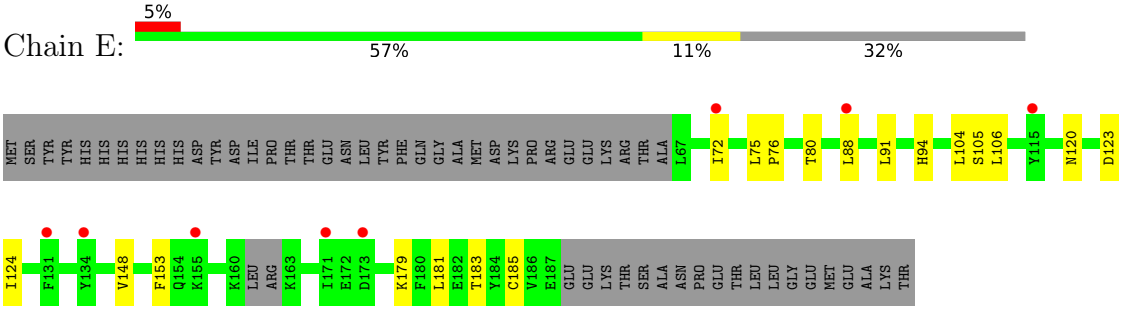
• Molecule 1: Regulator of nonsense transcripts 3A

Chain A:



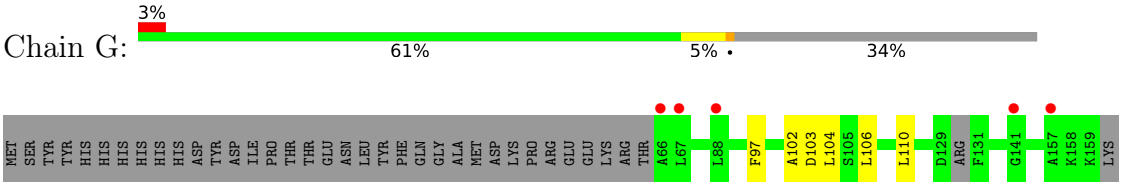
• Molecule 1: Regulator of nonsense transcripts 3A

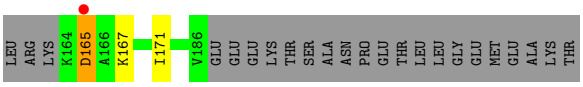
Chain E:



• Molecule 1: Regulator of nonsense transcripts 3A

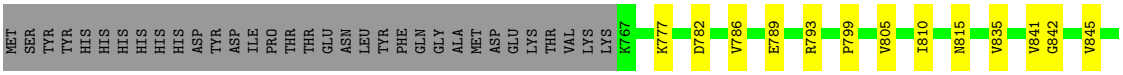
Chain G:

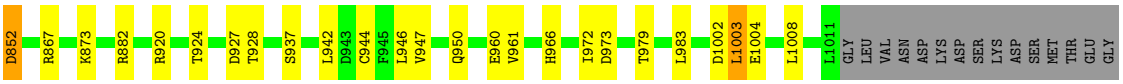


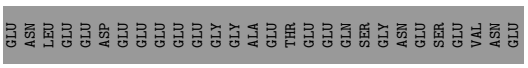


• Molecule 2: Regulator of nonsense transcripts 2

Chain D:

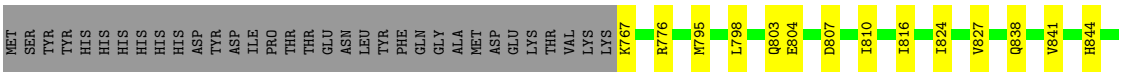


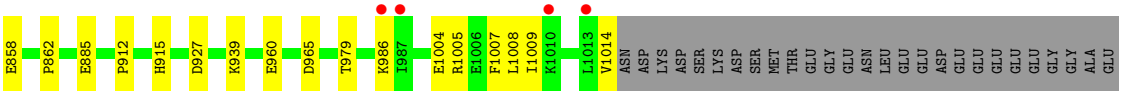


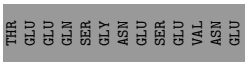


• Molecule 2: Regulator of nonsense transcripts 2

Chain B:

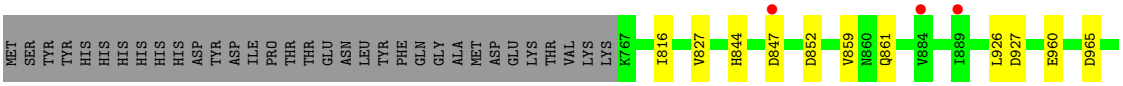


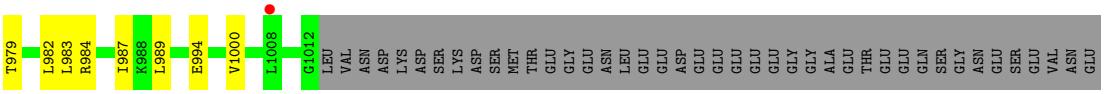




• Molecule 2: Regulator of nonsense transcripts 2

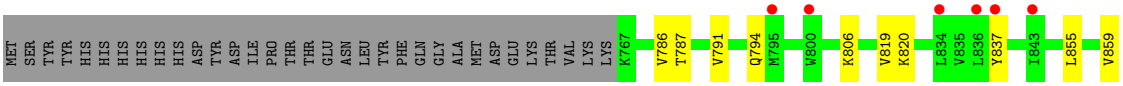
Chain F:

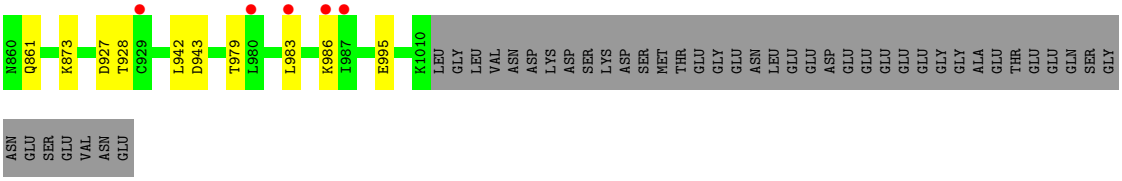




• Molecule 2: Regulator of nonsense transcripts 2

Chain H:




N860
Q861
K873
D927
T928
C929
L942
D943
T979
L980
L983
K986
I987
E995
K1010
LEU GLY LEU VAL ASN ASP LYS ASP SER LYS ASP SER MET THR GLU GLY GLU ASN LEU GLU GLU ASP GLU GLU GLU GLU GLY GLY ALA GLU THR GLU GLU GLN SER GLY
ASN GLU SER GLU VAL ASN GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.68Å 108.58Å 119.94Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	65.25 – 2.95 65.25 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (65.25-2.95) 98.6 (65.25-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.207 , 0.263 0.214 , 0.264	Depositor DCC
R_{free} test set	2080 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.178 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11757	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.26	0/992	0.48	0/1351
1	C	0.26	0/955	0.46	0/1300
1	E	0.27	0/930	0.45	0/1269
1	G	0.27	0/927	0.47	0/1265
2	B	0.25	0/2080	0.46	0/2821
2	D	0.25	0/2061	0.46	0/2795
2	F	0.25	0/2033	0.45	0/2760
2	H	0.25	0/2021	0.44	0/2742
All	All	0.25	0/11999	0.46	0/16303

There are no bond length outliers.

There are no bond angle outliers.

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	965	0	882	12	0
1	C	928	0	865	3	0
1	E	904	0	806	12	0
1	G	901	0	823	5	0
2	B	2033	0	2022	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2015	0	1997	20	0
2	F	1987	0	1964	10	0
2	H	1974	0	1955	9	0
3	B	10	0	14	0	0
3	D	10	0	14	0	0
3	F	10	0	14	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	1	0
5	C	1	0	0	0	0
5	D	9	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	3	0	0	0	0
All	All	11757	0	11356	81	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 4.

The worst 5 of 81 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:H:873:LYS:HD2	2:H:928:THR:HG21	1.71	0.70
2:D:920[B]:ARG:NH1	2:D:972:ILE:HD11	2.09	0.68
2:D:927:ASP:OD1	2:D:979:THR:HG22	1.96	0.65
2:D:942:LEU:HD21	2:D:983:LEU:HD23	1.79	0.65
2:B:776:ARG:NH1	5:B:1201:HOH:O	2.30	0.65

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	119/176 (68%)	109 (92%)	10 (8%)	0	100	100
1	C	113/176 (64%)	106 (94%)	7 (6%)	0	100	100
1	E	115/176 (65%)	102 (89%)	13 (11%)	0	100	100
1	G	110/176 (62%)	101 (92%)	9 (8%)	0	100	100
2	B	247/321 (77%)	234 (95%)	13 (5%)	0	100	100
2	D	244/321 (76%)	233 (96%)	11 (4%)	0	100	100
2	F	244/321 (76%)	234 (96%)	10 (4%)	0	100	100
2	H	242/321 (75%)	228 (94%)	14 (6%)	0	100	100
All	All	1434/1988 (72%)	1347 (94%)	87 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	94/158 (60%)	92 (98%)	2 (2%)	53	80
1	C	93/158 (59%)	92 (99%)	1 (1%)	73	89
1	E	86/158 (54%)	83 (96%)	3 (4%)	36	68
1	G	88/158 (56%)	85 (97%)	3 (3%)	37	69
2	B	226/300 (75%)	220 (97%)	6 (3%)	44	74
2	D	224/300 (75%)	214 (96%)	10 (4%)	27	61
2	F	219/300 (73%)	215 (98%)	4 (2%)	59	82
2	H	216/300 (72%)	209 (97%)	7 (3%)	39	71
All	All	1246/1832 (68%)	1210 (97%)	36 (3%)	42	73

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	165	ASP
2	H	995	GLU

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Mol	Chain	Res	Type
2	H	806	LYS
2	H	927	ASP
1	A	106	LEU

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

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)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PGE	D	1101	-	9,9,9	0.51	0	8,8,8	0.21	0
3	PGE	B	1101	-	9,9,9	0.52	0	8,8,8	0.25	0
3	PGE	F	1101	-	9,9,9	0.50	0	8,8,8	0.36	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
3	PGE	D	1101	-	-	3/7/7/7	-
3	PGE	B	1101	-	-	2/7/7/7	-
3	PGE	F	1101	-	-	7/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1101	PGE	O2-C3-C4-O3
3	F	1101	PGE	O3-C5-C6-O4
3	F	1101	PGE	C4-C3-O2-C2
3	B	1101	PGE	O3-C5-C6-O4
3	D	1101	PGE	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	123/176 (69%)	-0.13	3 (2%) 59 42	43, 72, 96, 101	0
1	C	117/176 (66%)	-0.30	0 100 100	45, 79, 101, 117	0
1	E	119/176 (67%)	0.25	8 (6%) 17 10	57, 86, 103, 116	0
1	G	116/176 (65%)	-0.02	6 (5%) 27 17	52, 85, 102, 111	0
2	B	248/321 (77%)	-0.06	4 (1%) 72 55	28, 53, 80, 94	0
2	D	245/321 (76%)	-0.11	0 100 100	33, 57, 84, 100	0
2	F	246/321 (76%)	-0.12	4 (1%) 72 55	31, 60, 86, 101	0
2	H	244/321 (76%)	0.14	11 (4%) 33 21	47, 71, 91, 106	0
All	All	1458/1988 (73%)	-0.04	36 (2%) 57 40	28, 68, 95, 117	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	929	CYS	4.9
1	G	66	ALA	4.8
2	H	987	ILE	3.8
1	E	155	LYS	3.6
2	H	983	LEU	3.5

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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGE	B	1101	10/10	0.89	0.31	51,72,87,88	0
3	PGE	D	1101	10/10	0.91	0.19	59,67,74,78	0
3	PGE	F	1101	10/10	0.93	0.15	52,66,77,87	0
4	CL	F	1102	1/1	0.99	0.20	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.