wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:54 PM GMT

PDB ID	:	4DPG
Title	:	Crystal Structure of Human LysRS: P38/AIMP2 Complex I
Authors	:	Fang, P.; Wang, J.; Bennett, S.P.; Guo, M.
Deposited on	:	2012-02-13
Resolution	:	2.84 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

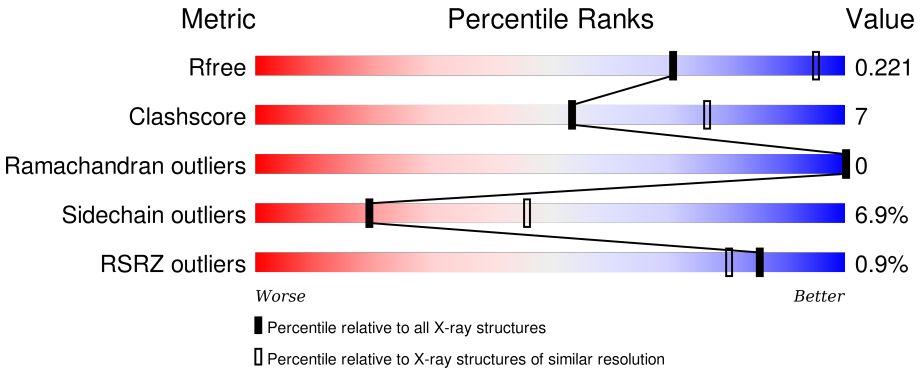
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.84 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}	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	77% 18%
1	B	513	83% 14%
1	C	513	% 75% 19%
1	D	513	% 80% 16%
1	E	513	78% 17%

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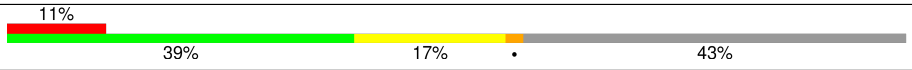
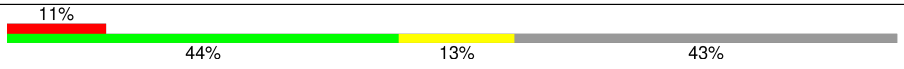
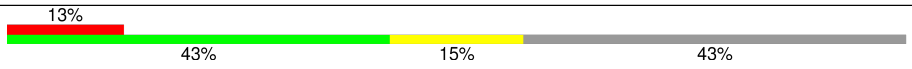
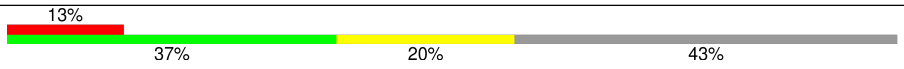
Mol	Chain	Length	Quality of chain
1	F	513	
1	G	513	
1	H	513	
2	I	54	
2	J	54	
2	K	54	
2	L	54	

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
4	APC	A	602	-	-	-	X
4	APC	B	602	-	-	-	X
4	APC	C	602	-	-	-	X
4	APC	D	602	-	-	-	X
4	APC	E	602	-	-	-	X
4	APC	F	602	-	-	-	X
4	APC	G	602	-	-	-	X
4	APC	H	603	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33740 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 Lysine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3932	2519	668	718	27			
1	B	506	Total	C	N	O	S	0	0	0
			4055	2596	687	744	28			
1	C	501	Total	C	N	O	S	0	0	0
			3989	2553	677	731	28			
1	D	505	Total	C	N	O	S	0	0	0
			4031	2588	685	730	28			
1	E	500	Total	C	N	O	S	0	0	0
			3969	2540	671	730	28			
1	F	505	Total	C	N	O	S	0	0	0
			4023	2580	685	730	28			
1	G	501	Total	C	N	O	S	0	0	0
			3921	2507	667	719	28			
1	H	505	Total	C	N	O	S	0	0	0
			4045	2590	685	742	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MET	-	EXPRESSION TAG	UNP Q15046
B	69	MET	-	EXPRESSION TAG	UNP Q15046
C	69	MET	-	EXPRESSION TAG	UNP Q15046
D	69	MET	-	EXPRESSION TAG	UNP Q15046
E	69	MET	-	EXPRESSION TAG	UNP Q15046
F	69	MET	-	EXPRESSION TAG	UNP Q15046
G	69	MET	-	EXPRESSION TAG	UNP Q15046
H	69	MET	-	EXPRESSION TAG	UNP Q15046

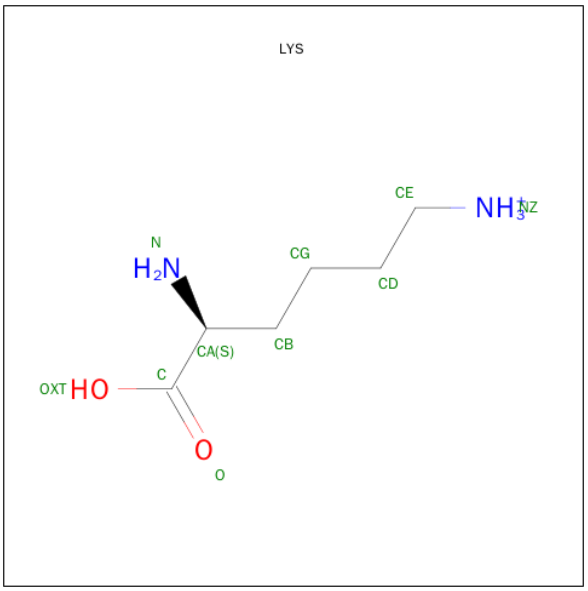
- Molecule 2 is a protein called Aminoacyl tRNA synthase complex-interacting multifunctional protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	31	Total	C	N	O	S	0	0	0
			224	144	40	37	3			
2	J	31	Total	C	N	O	S	0	0	0
			226	146	40	37	3			
2	K	31	Total	C	N	O	S	0	0	0
			224	144	40	37	3			
2	L	31	Total	C	N	O	S	0	0	0
			230	148	40	39	3			

There are 24 discrepancies between the modelled and reference sequences:

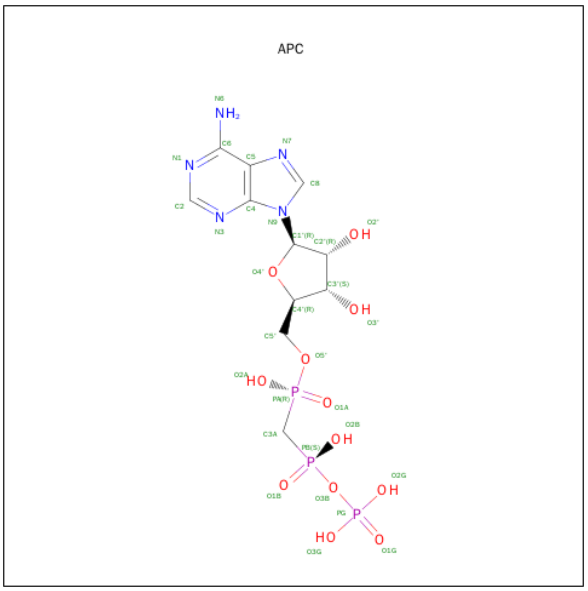
Chain	Residue	Modelled	Actual	Comment	Reference
I	49	HIS	-	EXPRESSION TAG	UNP Q13155
I	50	HIS	-	EXPRESSION TAG	UNP Q13155
I	51	HIS	-	EXPRESSION TAG	UNP Q13155
I	52	HIS	-	EXPRESSION TAG	UNP Q13155
I	53	HIS	-	EXPRESSION TAG	UNP Q13155
I	54	HIS	-	EXPRESSION TAG	UNP Q13155
J	49	HIS	-	EXPRESSION TAG	UNP Q13155
J	50	HIS	-	EXPRESSION TAG	UNP Q13155
J	51	HIS	-	EXPRESSION TAG	UNP Q13155
J	52	HIS	-	EXPRESSION TAG	UNP Q13155
J	53	HIS	-	EXPRESSION TAG	UNP Q13155
J	54	HIS	-	EXPRESSION TAG	UNP Q13155
K	49	HIS	-	EXPRESSION TAG	UNP Q13155
K	50	HIS	-	EXPRESSION TAG	UNP Q13155
K	51	HIS	-	EXPRESSION TAG	UNP Q13155
K	52	HIS	-	EXPRESSION TAG	UNP Q13155
K	53	HIS	-	EXPRESSION TAG	UNP Q13155
K	54	HIS	-	EXPRESSION TAG	UNP Q13155
L	49	HIS	-	EXPRESSION TAG	UNP Q13155
L	50	HIS	-	EXPRESSION TAG	UNP Q13155
L	51	HIS	-	EXPRESSION TAG	UNP Q13155
L	52	HIS	-	EXPRESSION TAG	UNP Q13155
L	53	HIS	-	EXPRESSION TAG	UNP Q13155
L	54	HIS	-	EXPRESSION TAG	UNP Q13155

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 6 2 2	0	0
3	B	1	Total C N O 10 6 2 2	0	0
3	C	1	Total C N O 10 6 2 2	0	0
3	D	1	Total C N O 10 6 2 2	0	0
3	E	1	Total C N O 10 6 2 2	0	0
3	F	1	Total C N O 10 6 2 2	0	0
3	G	1	Total C N O 10 6 2 2	0	0
3	H	1	Total C N O 10 6 2 2	0	0

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 27 11 5 9 2	0	0
4	B	1	Total C N O P 31 11 5 12 3	0	0
4	C	1	Total C N O P 27 11 5 9 2	0	0
4	D	1	Total C N O P 31 11 5 12 3	0	0
4	E	1	Total C N O P 27 11 5 9 2	0	0
4	F	1	Total C N O P 31 11 5 12 3	0	0
4	G	1	Total C N O P 27 11 5 9 2	0	0
4	H	1	Total C N O P 31 11 5 12 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

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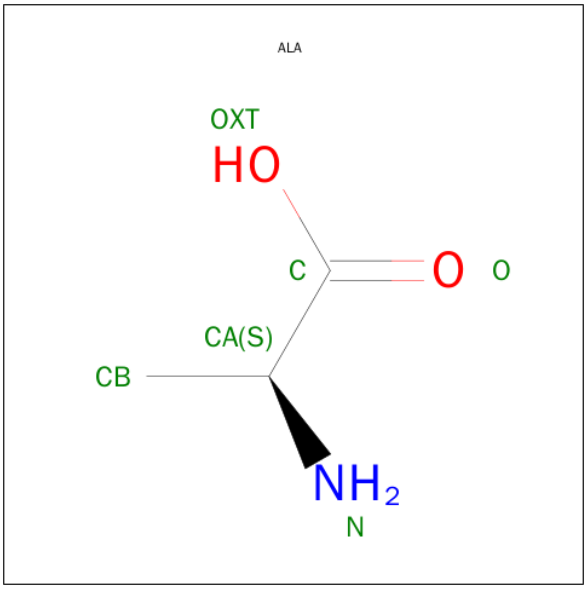
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	2	Total Mg 2 2	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	L	1	Total Mg 1 1	0	0
5	F	2	Total Mg 2 2	0	0

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C N O 5 3 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	47	Total O 47 47	0	0
7	B	85	Total O 85 85	0	0

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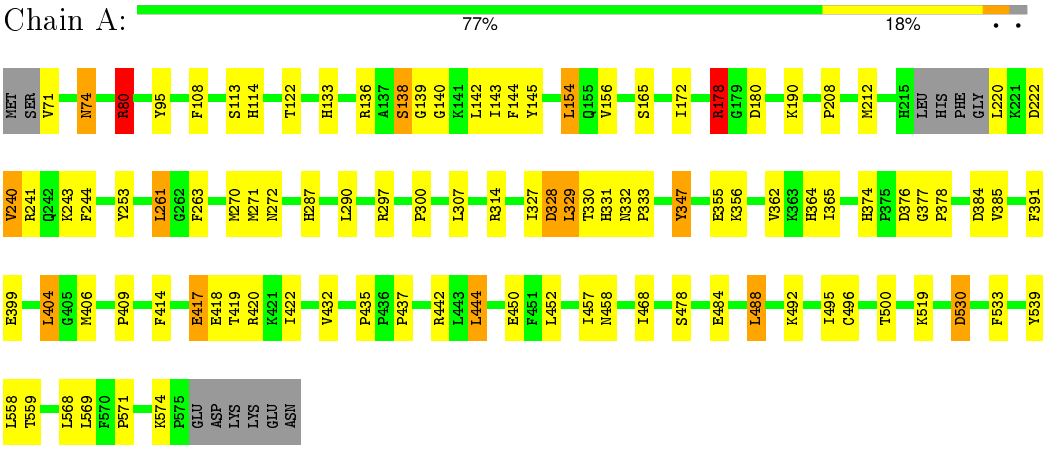
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	55	Total O 55 55	0	0
7	D	71	Total O 71 71	0	0
7	E	66	Total O 66 66	0	0
7	F	81	Total O 81 81	0	0
7	G	43	Total O 43 43	0	0
7	H	62	Total O 62 62	0	0
7	I	6	Total O 6 6	0	0
7	J	3	Total O 3 3	0	0
7	K	10	Total O 10 10	0	0
7	L	13	Total O 13 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

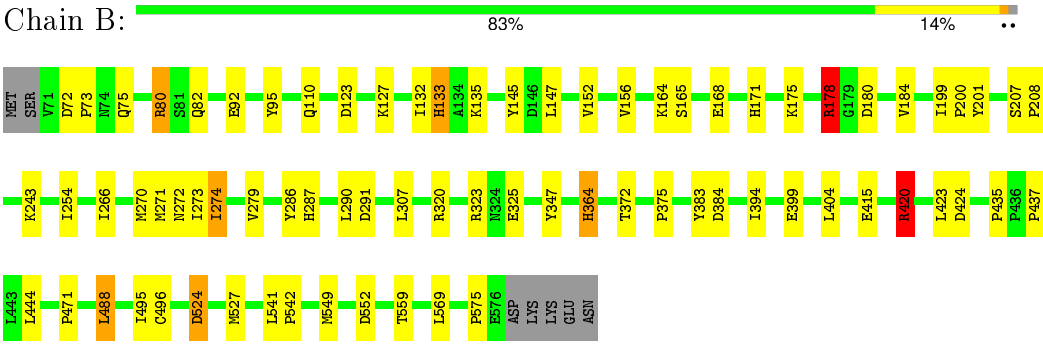
- Molecule 1: Lysine–tRNA ligase

Chain A:



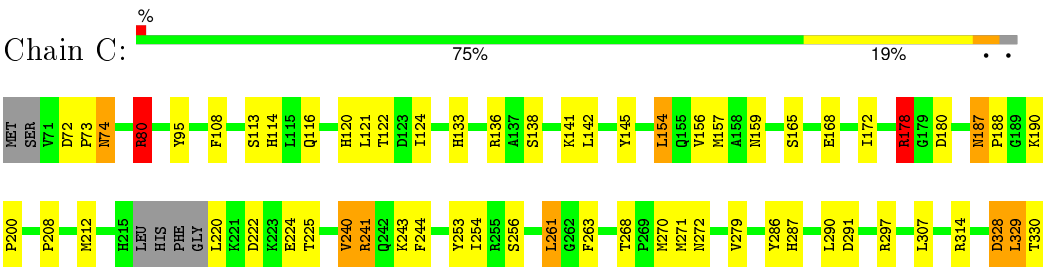
- Molecule 1: Lysine–tRNA ligase

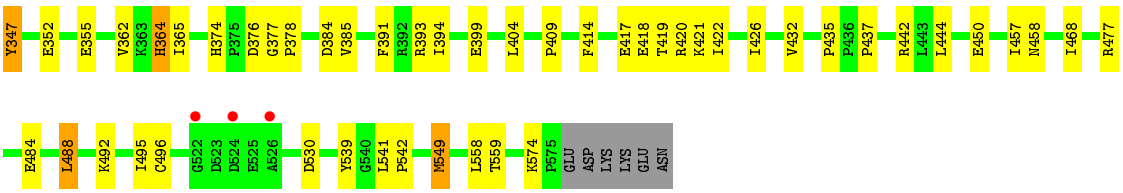
Chain B:



- Molecule 1: Lysine–tRNA ligase

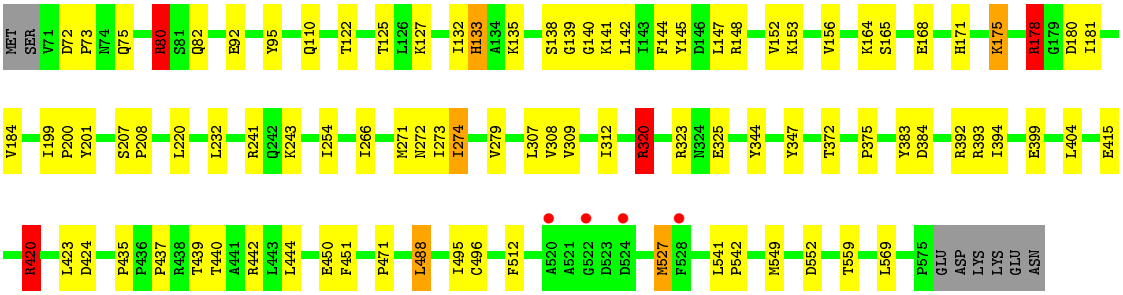
Chain C:





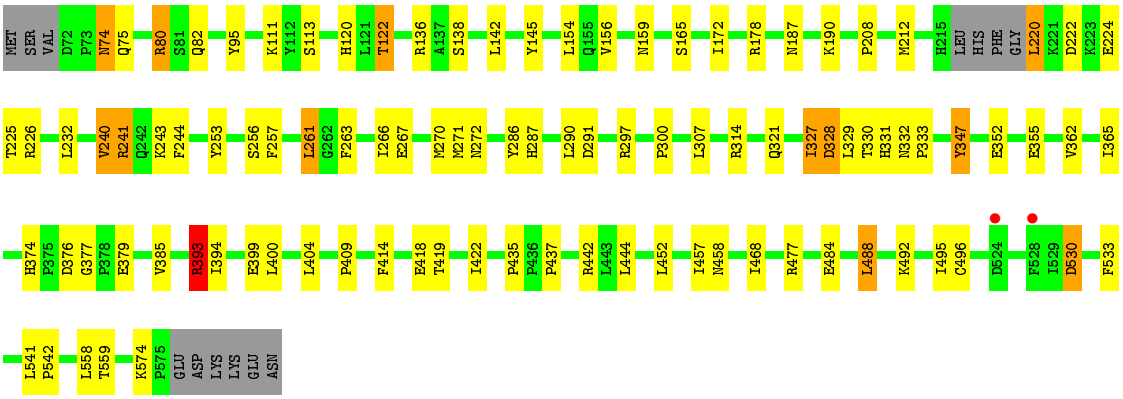
• Molecule 1: Lysine–tRNA ligase

Chain D:



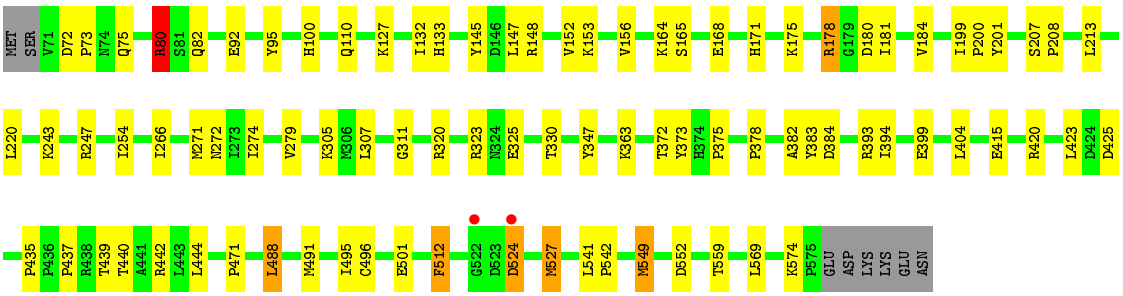
• Molecule 1: Lysine–tRNA ligase

Chain E:



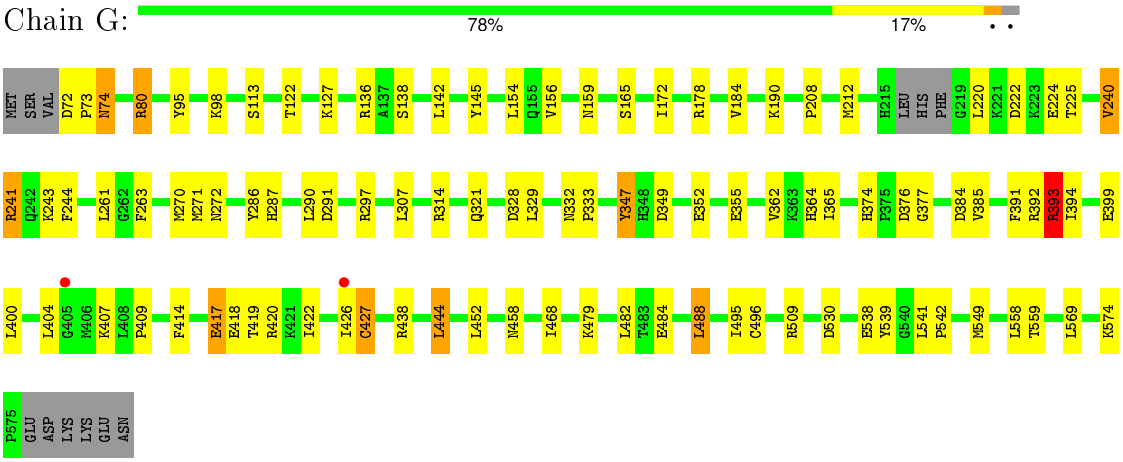
• Molecule 1: Lysine–tRNA ligase

Chain F:



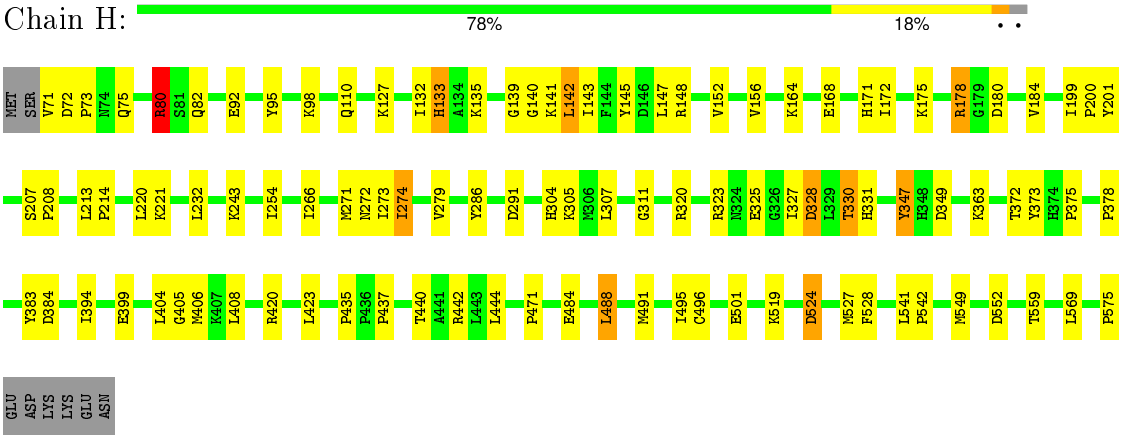
• Molecule 1: Lysine–tRNA ligase

Chain G:



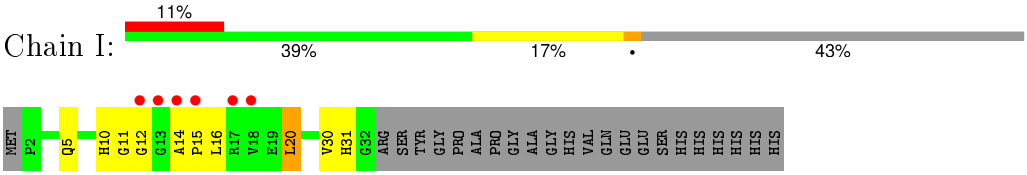
• Molecule 1: Lysine–tRNA ligase

Chain H:



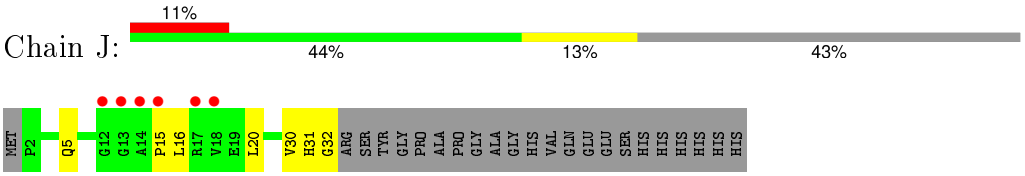
• Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain I:



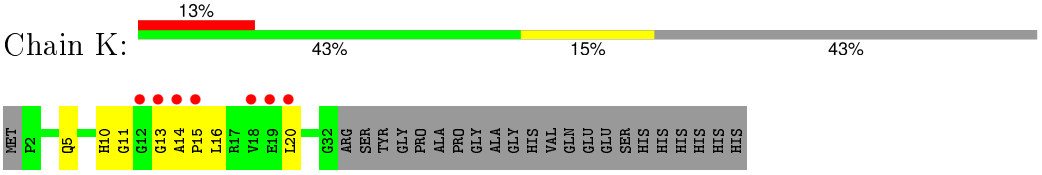
• Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain J:



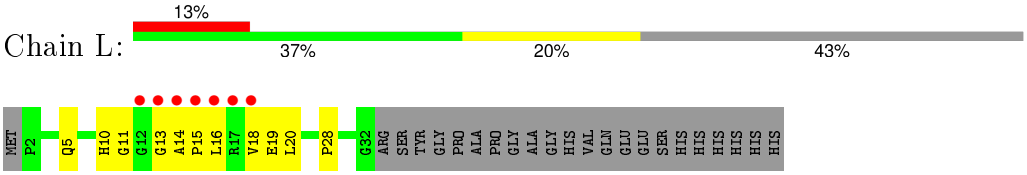
• Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain K:



• Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	79.20Å 122.01Å 149.20Å 89.16° 85.58° 89.71°	Depositor
Resolution (Å)	46.84 – 2.84 47.84 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.84-2.84) 95.8 (47.84-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.185 , 0.223 0.186 , 0.221	Depositor DCC
R_{free} test set	6481 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 14.9	EDS
Estimated twinning fraction	0.339 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 128809 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33740	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: APC, MG

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	0.51	0/4025	0.82	12/5457 (0.2%)
1	B	0.50	0/4152	0.75	10/5619 (0.2%)
1	C	0.48	0/4082	0.72	12/5526 (0.2%)
1	D	0.52	0/4128	0.91	14/5586 (0.3%)
1	E	0.48	0/4062	0.81	14/5503 (0.3%)
1	F	0.50	0/4120	0.73	12/5577 (0.2%)
1	G	0.49	0/4012	0.72	10/5440 (0.2%)
1	H	0.51	0/4142	0.73	10/5607 (0.2%)
2	I	0.49	0/233	0.78	0/319
2	J	0.60	0/235	0.75	0/322
2	K	0.58	0/233	0.78	0/319
2	L	0.57	0/239	0.67	0/327
All	All	0.50	0/33663	0.77	94/45602 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	E	0	1
1	G	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	320	ARG	NE-CZ-NH2	21.80	131.20	120.30
1	A	241	ARG	NE-CZ-NH2	20.63	130.61	120.30
1	D	393	ARG	NE-CZ-NH2	19.46	130.03	120.30
1	D	320	ARG	NE-CZ-NH1	-19.00	110.80	120.30
1	E	477	ARG	NE-CZ-NH1	18.84	129.72	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	574	LYS	Peptide
1	B	575	PRO	Peptide
1	C	574	LYS	Peptide
1	E	574	LYS	Peptide
1	G	574	LYS	Peptide

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	3932	0	3804	59	0
1	B	4055	0	3984	41	0
1	C	3989	0	3910	72	0
1	D	4031	0	3977	51	0
1	E	3969	0	3873	61	0
1	F	4023	0	3964	42	0
1	G	3921	0	3801	47	0
1	H	4045	0	3981	61	0
2	I	224	0	200	6	0
2	J	226	0	207	3	0
2	K	224	0	200	12	0
2	L	230	0	211	15	0
3	A	10	0	12	0	0
3	B	10	0	12	0	0
3	C	10	0	12	0	0
3	D	10	0	12	0	0
3	E	10	0	12	0	0
3	F	10	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	10	0	12	0	0
3	H	10	0	12	0	0
4	A	27	0	14	1	0
4	B	31	0	14	0	0
4	C	27	0	14	1	0
4	D	31	0	14	0	0
4	E	27	0	14	2	0
4	F	31	0	14	0	0
4	G	27	0	14	0	0
4	H	31	0	14	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
6	H	5	0	4	1	0
7	A	47	0	0	2	0
7	B	85	0	0	3	0
7	C	55	0	0	4	0
7	D	71	0	0	3	0
7	E	66	0	0	1	0
7	F	81	0	0	2	0
7	G	43	0	0	1	0
7	H	62	0	0	3	0
7	I	6	0	0	0	0
7	J	3	0	0	0	0
7	K	10	0	0	0	0
7	L	13	0	0	1	0
All	All	33740	0	32324	428	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 7.

The worst 5 of 428 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:270:MET:HE3	7:C:739:HOH:O	1.63	0.97
1:C:124:ILE:O	1:C:187:ASN:HB3	1.68	0.92
7:B:776:HOH:O	2:I:14:ALA:HB2	1.72	0.88
1:C:256:SER:OG	2:K:14:ALA:HB1	1.73	0.88
1:G:427:CYS:SG	1:G:438:ARG:NH1	2.51	0.84

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	497/513 (97%)	477 (96%)	20 (4%)	0	100	100
1	B	504/513 (98%)	495 (98%)	9 (2%)	0	100	100
1	C	497/513 (97%)	479 (96%)	18 (4%)	0	100	100
1	D	503/513 (98%)	493 (98%)	10 (2%)	0	100	100
1	E	496/513 (97%)	478 (96%)	18 (4%)	0	100	100
1	F	503/513 (98%)	495 (98%)	8 (2%)	0	100	100
1	G	497/513 (97%)	477 (96%)	20 (4%)	0	100	100
1	H	503/513 (98%)	493 (98%)	10 (2%)	0	100	100
2	I	29/54 (54%)	25 (86%)	4 (14%)	0	100	100
2	J	29/54 (54%)	24 (83%)	5 (17%)	0	100	100
2	K	29/54 (54%)	23 (79%)	6 (21%)	0	100	100
2	L	29/54 (54%)	26 (90%)	3 (10%)	0	100	100
All	All	4116/4320 (95%)	3985 (97%)	131 (3%)	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	409/455 (90%)	376 (92%)	33 (8%)	15 37
1	B	435/455 (96%)	411 (94%)	24 (6%)	27 58
1	C	425/455 (93%)	390 (92%)	35 (8%)	14 37
1	D	430/455 (94%)	405 (94%)	25 (6%)	25 55
1	E	422/455 (93%)	391 (93%)	31 (7%)	17 43
1	F	430/455 (94%)	404 (94%)	26 (6%)	24 54
1	G	410/455 (90%)	378 (92%)	32 (8%)	16 39
1	H	436/455 (96%)	410 (94%)	26 (6%)	24 54
2	I	21/44 (48%)	18 (86%)	3 (14%)	4 11
2	J	22/44 (50%)	19 (86%)	3 (14%)	5 13
2	K	21/44 (48%)	20 (95%)	1 (5%)	31 64
2	L	23/44 (52%)	20 (87%)	3 (13%)	5 14
All	All	3484/3816 (91%)	3242 (93%)	242 (7%)	19 46

5 of 242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	347	TYR
1	E	272	ASN
1	H	327	ILE
1	D	420	ARG
1	E	122	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	120	HIS
1	E	187	ASN
1	G	287	HIS
1	C	364	HIS

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Mol	Chain	Res	Type
1	G	187	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 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	LYS	A	601	-	6,9,9	0.28	0	4,10,10	0.46	0
4	APC	A	602	-	22,29,33	1.52	5 (22%)	27,45,52	2.27	3 (11%)
3	LYS	B	601	-	6,9,9	0.32	0	4,10,10	0.42	0
4	APC	B	602	5	25,33,33	1.62	6 (24%)	30,52,52	2.12	5 (16%)
3	LYS	C	601	-	6,9,9	0.37	0	4,10,10	0.48	0
4	APC	C	602	-	22,29,33	1.54	5 (22%)	27,45,52	2.32	3 (11%)
3	LYS	D	601	-	6,9,9	0.49	0	4,10,10	0.41	0
4	APC	D	602	5	25,33,33	1.64	6 (24%)	30,52,52	2.11	4 (13%)
3	LYS	E	601	-	6,9,9	0.38	0	4,10,10	0.43	0
4	APC	E	602	-	22,29,33	1.53	5 (22%)	27,45,52	2.32	3 (11%)
3	LYS	F	601	-	6,9,9	0.41	0	4,10,10	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	APC	F	602	5	25,33,33	1.63	5 (20%)	30,52,52	2.23	4 (13%)
3	LYS	G	601	-	6,9,9	0.34	0	4,10,10	0.51	0
4	APC	G	602	-	22,29,33	1.57	5 (22%)	27,45,52	2.27	3 (11%)
6	ALA	H	601	-	3,4,5	0.84	0	0,4,6	0.00	-
3	LYS	H	602	-	6,9,9	0.44	0	4,10,10	0.37	0
4	APC	H	603	5	25,33,33	1.59	6 (24%)	30,52,52	2.24	4 (13%)

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	LYS	A	601	-	-	0/5/9/9	0/0/0/0
4	APC	A	602	-	-	0/12/32/38	0/3/3/3
3	LYS	B	601	-	-	0/5/9/9	0/0/0/0
4	APC	B	602	5	-	0/15/38/38	0/3/3/3
3	LYS	C	601	-	-	0/5/9/9	0/0/0/0
4	APC	C	602	-	-	0/12/32/38	0/3/3/3
3	LYS	D	601	-	-	0/5/9/9	0/0/0/0
4	APC	D	602	5	-	0/15/38/38	0/3/3/3
3	LYS	E	601	-	-	0/5/9/9	0/0/0/0
4	APC	E	602	-	-	0/12/32/38	0/3/3/3
3	LYS	F	601	-	-	0/5/9/9	0/0/0/0
4	APC	F	602	5	-	0/15/38/38	0/3/3/3
3	LYS	G	601	-	-	0/5/9/9	0/0/0/0
4	APC	G	602	-	-	0/12/32/38	0/3/3/3
6	ALA	H	601	-	-	0/0/2/4	0/0/0/0
3	LYS	H	602	-	-	0/5/9/9	0/0/0/0
4	APC	H	603	5	-	0/15/38/38	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	603	APC	PB-O2B	2.04	1.61	1.56
4	D	602	APC	PA-O2A	2.04	1.61	1.56
4	B	602	APC	PA-O2A	2.05	1.61	1.56
4	H	603	APC	PA-O2A	2.08	1.61	1.56
4	B	602	APC	PB-O2B	2.13	1.61	1.56

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	602	APC	N3-C2-N1	-10.39	120.94	128.89
4	E	602	APC	N3-C2-N1	-10.36	120.96	128.89
4	A	602	APC	N3-C2-N1	-10.17	121.11	128.89
4	G	602	APC	N3-C2-N1	-10.16	121.12	128.89
4	H	603	APC	N3-C2-N1	-10.08	121.17	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	APC	1	0
4	C	602	APC	1	0
4	E	602	APC	2	0
6	H	601	ALA	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	501/513 (97%)	-0.34	0 100 100	17, 49, 84, 100	0
1	B	506/513 (98%)	-0.56	0 100 100	17, 33, 66, 82	0
1	C	501/513 (97%)	-0.47	3 (0%) 90 87	16, 40, 74, 97	0
1	D	505/513 (98%)	-0.49	4 (0%) 87 82	16, 34, 70, 112	0
1	E	500/513 (97%)	-0.50	2 (0%) 93 90	16, 39, 75, 114	0
1	F	505/513 (98%)	-0.53	2 (0%) 93 90	16, 33, 72, 117	0
1	G	501/513 (97%)	-0.35	2 (0%) 93 90	19, 49, 83, 108	0
1	H	505/513 (98%)	-0.46	0 100 100	18, 33, 65, 91	0
2	I	31/54 (57%)	0.56	6 (19%) 1 1	23, 50, 114, 118	0
2	J	31/54 (57%)	0.75	6 (19%) 1 1	21, 53, 115, 125	0
2	K	31/54 (57%)	0.85	7 (22%) 1 1	21, 53, 113, 118	0
2	L	31/54 (57%)	0.95	7 (22%) 1 1	20, 49, 114, 116	0
All	All	4148/4320 (96%)	-0.43	39 (0%) 85 80	16, 37, 79, 125	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	12	GLY	8.4
2	J	14	ALA	8.3
2	L	13	GLY	8.1
1	D	524	ASP	6.7
2	J	12	GLY	6.3

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 (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	APC	A	602	27/31	0.80	0.42	7.24	73,101,138,154	0
4	APC	G	602	27/31	0.75	0.41	6.05	83,111,142,148	0
4	APC	B	602	31/31	0.81	0.28	4.81	57,101,132,156	0
4	APC	H	603	31/31	0.80	0.29	4.34	56,105,139,158	0
4	APC	E	602	27/31	0.80	0.28	3.91	74,99,127,160	0
4	APC	F	602	31/31	0.79	0.28	2.79	61,107,145,155	0
4	APC	C	602	27/31	0.78	0.34	2.77	72,101,131,155	0
4	APC	D	602	31/31	0.81	0.27	2.16	60,108,149,152	0
3	LYS	C	601	10/10	0.96	0.20	1.14	15,19,42,44	0
3	LYS	A	601	10/10	0.97	0.19	0.96	16,24,46,61	0
3	LYS	G	601	10/10	0.95	0.17	0.53	17,33,43,52	0
3	LYS	H	602	10/10	0.97	0.16	0.52	18,22,30,32	0
3	LYS	B	601	10/10	0.97	0.15	0.50	15,24,32,35	0
3	LYS	D	601	10/10	0.96	0.15	0.19	15,31,36,38	0
3	LYS	F	601	10/10	0.96	0.15	-0.31	17,30,36,39	0
3	LYS	E	601	10/10	0.97	0.14	-0.81	15,22,45,49	0
5	MG	D	603	1/1	0.76	0.12	-	68,68,68,68	0
5	MG	F	604	1/1	0.96	0.21	-	12,12,12,12	0
5	MG	H	604	1/1	0.77	0.09	-	66,66,66,66	0
5	MG	C	603	1/1	0.94	0.15	-	59,59,59,59	0
5	MG	H	605	1/1	0.93	0.26	-	13,13,13,13	0
5	MG	E	603	1/1	0.95	0.09	-	53,53,53,53	0
5	MG	L	101	1/1	0.96	0.30	-	20,20,20,20	0
5	MG	B	603	1/1	0.77	0.17	-	63,63,63,63	0
6	ALA	H	601	5/6	0.73	0.20	-	69,76,79,80	0
5	MG	J	101	1/1	0.84	0.27	-	21,21,21,21	0
5	MG	F	603	1/1	0.72	0.09	-	59,59,59,59	0
5	MG	A	603	1/1	0.89	0.09	-	53,53,53,53	0
5	MG	G	603	1/1	0.93	0.12	-	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.