Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2022 – 10:40 am BST

PDB ID	:	7QYR
Title	:	Crystal structure of RimK from Pseudomonas aeruginosa PAO1
Authors	:	Thompson, C.M.A.; Little, R.H.; Stevenson, C.E.M.; Lawson, D.M.; Malone, J.G.
Deposited on	:	2022-01-29
Resolution	:	2.40 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 ⓘ 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 ⓘ) were used in the production of this report:

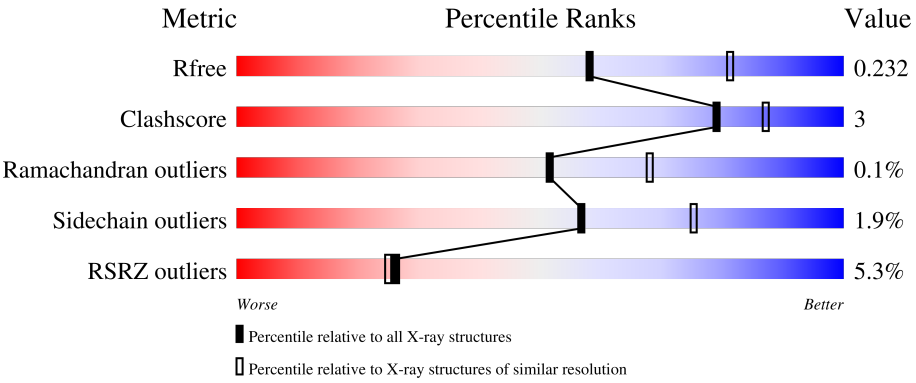
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	314	2% 86% 7% 7%
1	B	314	% 83% 9% 9%
1	C	314	2% 83% 7% 10%
1	D	314	6% 88% 5% 7%
1	E	314	86% 6% 8%

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Mol	Chain	Length	Quality of chain
1	F	314	9% 80% 7% 12%
1	G	314	8% 85% 6% 9%
1	H	314	6% 82% 7% 11%
2	K	60	7% 92%
2	L	60	2% 5% 92%
2	M	60	3% 7% 92%
2	N	60	3% 5% 95%
2	O	60	3% 5% 95%
2	P	60	2% 7% 92%
2	Q	60	3% 5% 92%
2	T	60	15% 37% 7% 57%

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
3	ADP	D	401	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17790 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 Probable alpha-L-glutamate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2184	1374	392	403	15			
1	B	287	Total	C	N	O	S	0	0	0
			2149	1356	382	396	15			
1	C	284	Total	C	N	O	S	0	0	0
			2124	1340	376	393	15			
1	D	293	Total	C	N	O	S	0	0	0
			2179	1373	388	403	15			
1	E	290	Total	C	N	O	S	0	0	0
			2163	1362	386	400	15			
1	F	277	Total	C	N	O	S	0	0	0
			2082	1312	370	386	14			
1	G	286	Total	C	N	O	S	0	0	0
			2130	1341	379	395	15			
1	H	279	Total	C	N	O	S	0	0	0
			2084	1315	366	388	15			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	LYS	-	expression tag	UNP Q9HTZ2
A	303	LEU	-	expression tag	UNP Q9HTZ2
A	304	ALA	-	expression tag	UNP Q9HTZ2
A	305	ALA	-	expression tag	UNP Q9HTZ2
A	306	ALA	-	expression tag	UNP Q9HTZ2
A	307	LEU	-	expression tag	UNP Q9HTZ2
A	308	GLU	-	expression tag	UNP Q9HTZ2
A	309	HIS	-	expression tag	UNP Q9HTZ2
A	310	HIS	-	expression tag	UNP Q9HTZ2
A	311	HIS	-	expression tag	UNP Q9HTZ2
A	312	HIS	-	expression tag	UNP Q9HTZ2
A	313	HIS	-	expression tag	UNP Q9HTZ2
A	314	HIS	-	expression tag	UNP Q9HTZ2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	LYS	-	expression tag	UNP Q9HTZ2
B	303	LEU	-	expression tag	UNP Q9HTZ2
B	304	ALA	-	expression tag	UNP Q9HTZ2
B	305	ALA	-	expression tag	UNP Q9HTZ2
B	306	ALA	-	expression tag	UNP Q9HTZ2
B	307	LEU	-	expression tag	UNP Q9HTZ2
B	308	GLU	-	expression tag	UNP Q9HTZ2
B	309	HIS	-	expression tag	UNP Q9HTZ2
B	310	HIS	-	expression tag	UNP Q9HTZ2
B	311	HIS	-	expression tag	UNP Q9HTZ2
B	312	HIS	-	expression tag	UNP Q9HTZ2
B	313	HIS	-	expression tag	UNP Q9HTZ2
B	314	HIS	-	expression tag	UNP Q9HTZ2
C	302	LYS	-	expression tag	UNP Q9HTZ2
C	303	LEU	-	expression tag	UNP Q9HTZ2
C	304	ALA	-	expression tag	UNP Q9HTZ2
C	305	ALA	-	expression tag	UNP Q9HTZ2
C	306	ALA	-	expression tag	UNP Q9HTZ2
C	307	LEU	-	expression tag	UNP Q9HTZ2
C	308	GLU	-	expression tag	UNP Q9HTZ2
C	309	HIS	-	expression tag	UNP Q9HTZ2
C	310	HIS	-	expression tag	UNP Q9HTZ2
C	311	HIS	-	expression tag	UNP Q9HTZ2
C	312	HIS	-	expression tag	UNP Q9HTZ2
C	313	HIS	-	expression tag	UNP Q9HTZ2
C	314	HIS	-	expression tag	UNP Q9HTZ2
D	302	LYS	-	expression tag	UNP Q9HTZ2
D	303	LEU	-	expression tag	UNP Q9HTZ2
D	304	ALA	-	expression tag	UNP Q9HTZ2
D	305	ALA	-	expression tag	UNP Q9HTZ2
D	306	ALA	-	expression tag	UNP Q9HTZ2
D	307	LEU	-	expression tag	UNP Q9HTZ2
D	308	GLU	-	expression tag	UNP Q9HTZ2
D	309	HIS	-	expression tag	UNP Q9HTZ2
D	310	HIS	-	expression tag	UNP Q9HTZ2
D	311	HIS	-	expression tag	UNP Q9HTZ2
D	312	HIS	-	expression tag	UNP Q9HTZ2
D	313	HIS	-	expression tag	UNP Q9HTZ2
D	314	HIS	-	expression tag	UNP Q9HTZ2
E	302	LYS	-	expression tag	UNP Q9HTZ2
E	303	LEU	-	expression tag	UNP Q9HTZ2
E	304	ALA	-	expression tag	UNP Q9HTZ2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	305	ALA	-	expression tag	UNP Q9HTZ2
E	306	ALA	-	expression tag	UNP Q9HTZ2
E	307	LEU	-	expression tag	UNP Q9HTZ2
E	308	GLU	-	expression tag	UNP Q9HTZ2
E	309	HIS	-	expression tag	UNP Q9HTZ2
E	310	HIS	-	expression tag	UNP Q9HTZ2
E	311	HIS	-	expression tag	UNP Q9HTZ2
E	312	HIS	-	expression tag	UNP Q9HTZ2
E	313	HIS	-	expression tag	UNP Q9HTZ2
E	314	HIS	-	expression tag	UNP Q9HTZ2
F	302	LYS	-	expression tag	UNP Q9HTZ2
F	303	LEU	-	expression tag	UNP Q9HTZ2
F	304	ALA	-	expression tag	UNP Q9HTZ2
F	305	ALA	-	expression tag	UNP Q9HTZ2
F	306	ALA	-	expression tag	UNP Q9HTZ2
F	307	LEU	-	expression tag	UNP Q9HTZ2
F	308	GLU	-	expression tag	UNP Q9HTZ2
F	309	HIS	-	expression tag	UNP Q9HTZ2
F	310	HIS	-	expression tag	UNP Q9HTZ2
F	311	HIS	-	expression tag	UNP Q9HTZ2
F	312	HIS	-	expression tag	UNP Q9HTZ2
F	313	HIS	-	expression tag	UNP Q9HTZ2
F	314	HIS	-	expression tag	UNP Q9HTZ2
G	302	LYS	-	expression tag	UNP Q9HTZ2
G	303	LEU	-	expression tag	UNP Q9HTZ2
G	304	ALA	-	expression tag	UNP Q9HTZ2
G	305	ALA	-	expression tag	UNP Q9HTZ2
G	306	ALA	-	expression tag	UNP Q9HTZ2
G	307	LEU	-	expression tag	UNP Q9HTZ2
G	308	GLU	-	expression tag	UNP Q9HTZ2
G	309	HIS	-	expression tag	UNP Q9HTZ2
G	310	HIS	-	expression tag	UNP Q9HTZ2
G	311	HIS	-	expression tag	UNP Q9HTZ2
G	312	HIS	-	expression tag	UNP Q9HTZ2
G	313	HIS	-	expression tag	UNP Q9HTZ2
G	314	HIS	-	expression tag	UNP Q9HTZ2
H	302	LYS	-	expression tag	UNP Q9HTZ2
H	303	LEU	-	expression tag	UNP Q9HTZ2
H	304	ALA	-	expression tag	UNP Q9HTZ2
H	305	ALA	-	expression tag	UNP Q9HTZ2
H	306	ALA	-	expression tag	UNP Q9HTZ2
H	307	LEU	-	expression tag	UNP Q9HTZ2

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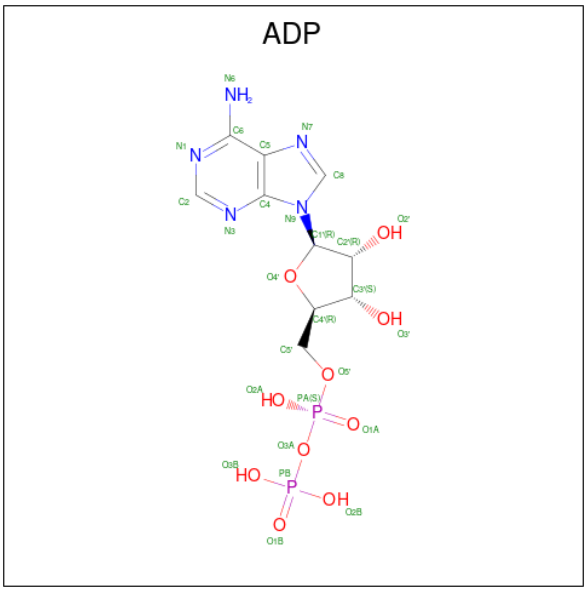
Chain	Residue	Modelled	Actual	Comment	Reference
H	308	GLU	-	expression tag	UNP Q9HTZ2
H	309	HIS	-	expression tag	UNP Q9HTZ2
H	310	HIS	-	expression tag	UNP Q9HTZ2
H	311	HIS	-	expression tag	UNP Q9HTZ2
H	312	HIS	-	expression tag	UNP Q9HTZ2
H	313	HIS	-	expression tag	UNP Q9HTZ2
H	314	HIS	-	expression tag	UNP Q9HTZ2

- Molecule 2 is a protein called poly-glutamate.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	K	5	Total C N O 37 21 5 11	0	0	0
2	L	5	Total C N O 37 21 5 11	0	0	0
2	M	5	Total C N O 37 21 5 11	0	0	0
2	N	3	Total C N O 23 13 3 7	0	0	0
2	O	3	Total C N O 23 13 3 7	0	0	0
2	P	5	Total C N O 37 21 5 11	0	0	0
2	Q	5	Total C N O 37 21 5 11	0	0	0
2	T	26	Total C N O 210 118 26 66	0	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 19 10 5 4	0	0
3	B	1	Total C N O 19 10 5 4	0	0
3	C	1	Total C N O 19 10 5 4	0	0
3	D	1	Total C N O 19 10 5 4	0	0
3	E	1	Total C N O 19 10 5 4	0	0
3	F	1	Total C N O 19 10 5 4	0	0
3	G	1	Total C N O 19 10 5 4	0	0
3	H	1	Total C N O 19 10 5 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	18	Total O 18 18	0	0
4	C	12	Total O 12 12	0	0
4	D	13	Total O 13 13	0	0

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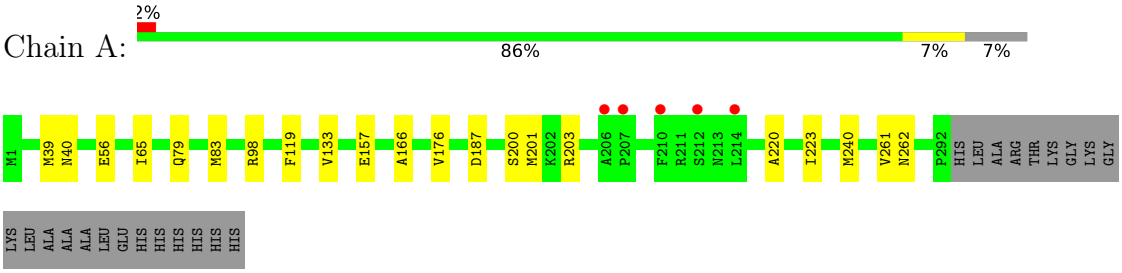
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	13	Total O 13 13	0	0
4	F	7	Total O 7 7	0	0
4	G	7	Total O 7 7	0	0
4	H	7	Total O 7 7	0	0

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.

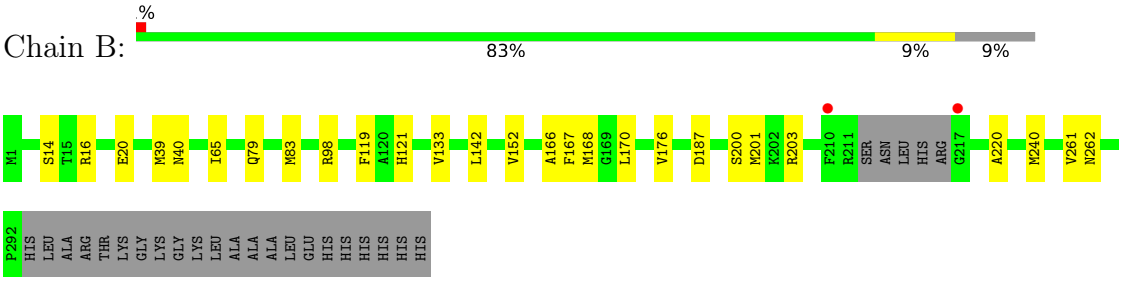
• Molecule 1: Probable alpha-L-glutamate ligase

Chain A:



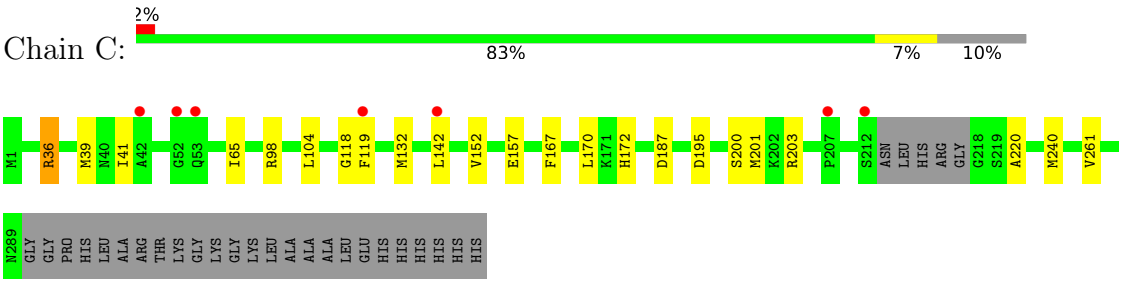
• Molecule 1: Probable alpha-L-glutamate ligase

Chain B:



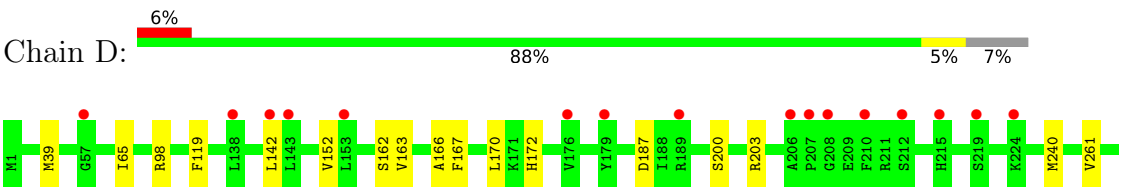
• Molecule 1: Probable alpha-L-glutamate ligase

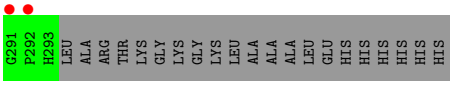
Chain C:



• Molecule 1: Probable alpha-L-glutamate ligase

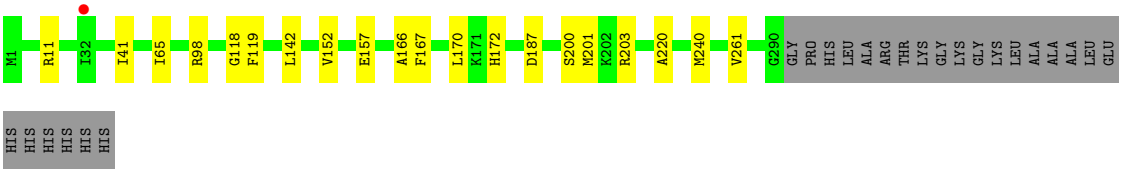
Chain D:





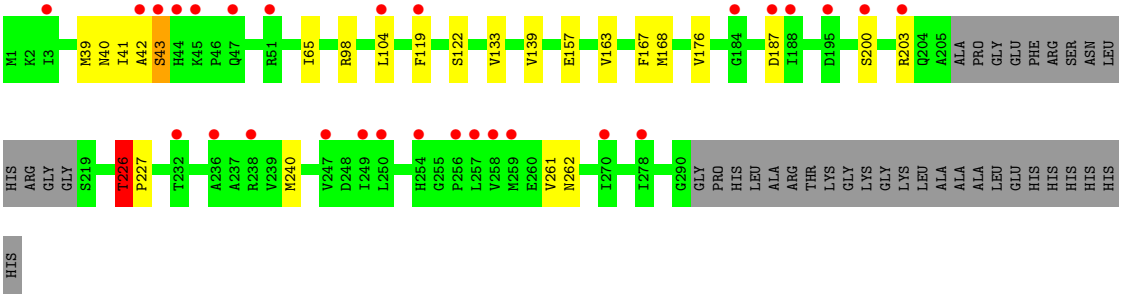
• Molecule 1: Probable alpha-L-glutamate ligase

Chain E:



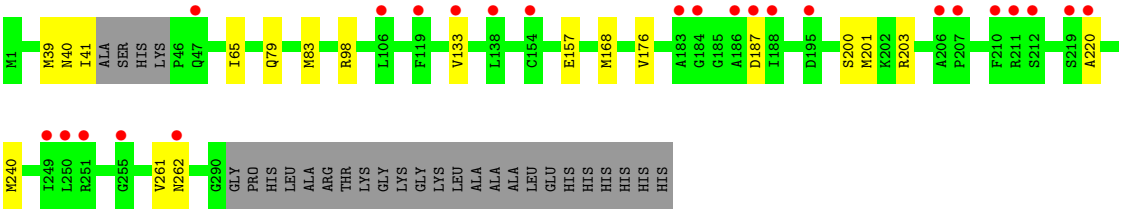
• Molecule 1: Probable alpha-L-glutamate ligase

Chain F:



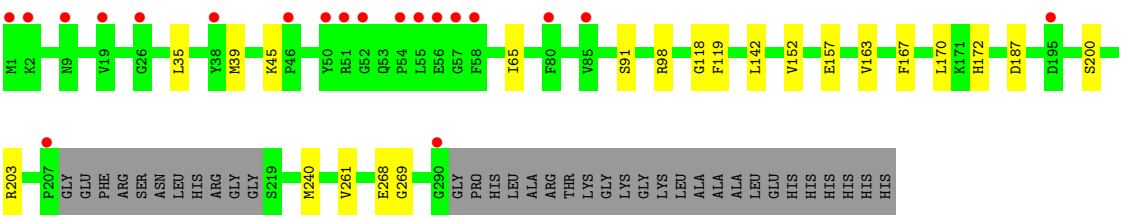
• Molecule 1: Probable alpha-L-glutamate ligase

Chain G:



• Molecule 1: Probable alpha-L-glutamate ligase

Chain H:

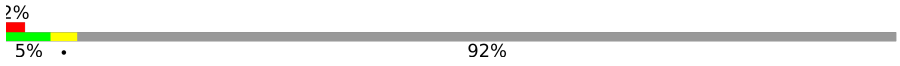


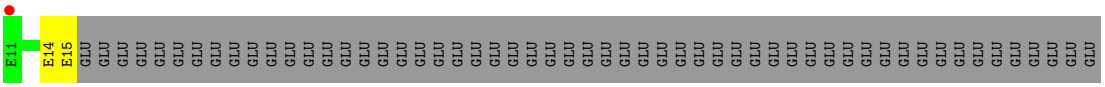
• Molecule 2: poly-glutamate

Chain K:

• Molecule 2: poly-glutamate

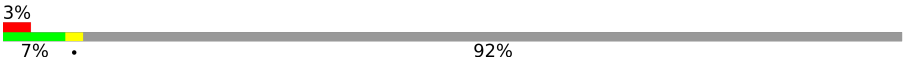
Chain L:





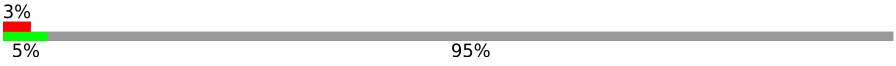
• Molecule 2: poly-glutamate

Chain M:



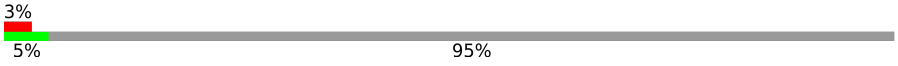
• Molecule 2: poly-glutamate

Chain N:



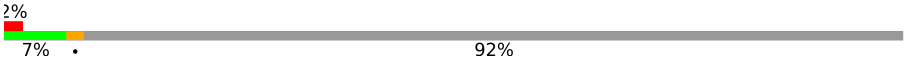
• Molecule 2: poly-glutamate

Chain O:



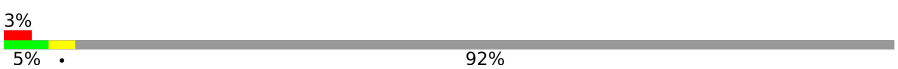
• Molecule 2: poly-glutamate

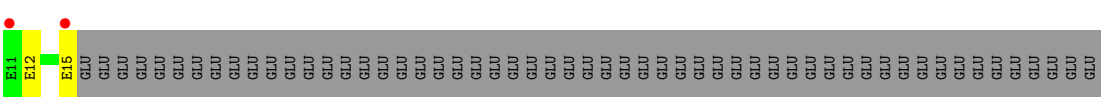
Chain P:



• Molecule 2: poly-glutamate

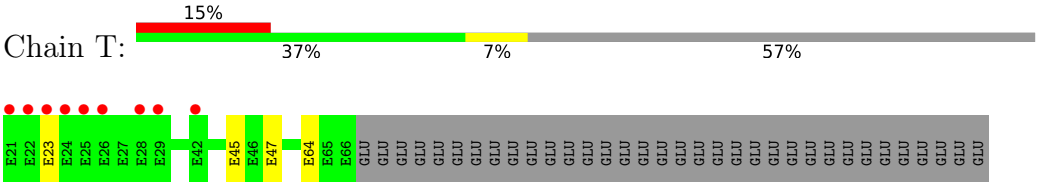
Chain Q:





• Molecule 2: poly-glutamate

Chain T:


15%
37%
7%
57%
E21
E22
E23
E24
E25
E26
E27
E28
E29
E42
E45
E46
E47
E64
E65
E66
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	66.90Å 153.59Å 138.54Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	44.45 – 2.40 44.41 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.45-2.40) 99.2 (44.41-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.232 0.213 , 0.232	Depositor DCC
R_{free} test set	5200 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17790	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: ADP

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	0.67	0/2217	0.78	0/2993
1	B	0.66	0/2181	0.78	0/2943
1	C	0.66	0/2154	0.78	1/2908 (0.0%)
1	D	0.68	0/2211	0.80	0/2985
1	E	0.66	0/2194	0.77	0/2962
1	F	0.66	0/2111	0.77	1/2851 (0.0%)
1	G	0.66	0/2160	0.76	0/2917
1	H	0.67	0/2113	0.79	0/2856
2	K	0.82	0/36	0.90	0/47
2	L	0.82	0/36	0.73	0/47
2	M	0.83	0/36	0.72	0/47
2	N	0.75	0/22	0.62	0/28
2	O	0.86	0/22	0.87	0/28
2	P	2.65	1/36 (2.8%)	0.77	0/47
2	Q	1.15	0/36	0.72	0/47
2	T	0.82	0/207	0.81	0/273
All	All	0.68	1/17772 (0.0%)	0.78	2/23979 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	15	GLU	C-O	15.11	1.52	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	36	ARG	CB-CG-CD	5.57	126.07	111.60
1	F	226	THR	CA-CB-OG1	5.10	119.71	109.00

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	2184	0	2228	14	0
1	B	2149	0	2196	23	0
1	C	2124	0	2168	18	0
1	D	2179	0	2221	10	0
1	E	2163	0	2202	13	0
1	F	2082	0	2123	21	0
1	G	2130	0	2155	11	0
1	H	2084	0	2119	12	0
2	K	37	0	21	2	0
2	L	37	0	21	3	0
2	M	37	0	21	0	0
2	N	23	0	13	0	0
2	O	23	0	13	0	0
2	P	37	0	21	1	0
2	Q	37	0	21	1	0
2	T	210	0	129	3	0
3	A	19	0	12	0	0
3	B	19	0	12	0	0
3	C	19	0	12	0	0
3	D	19	0	12	0	0
3	E	19	0	12	0	0
3	F	19	0	12	1	0
3	G	19	0	12	0	0
3	H	19	0	12	0	0
4	A	25	0	0	1	0
4	B	18	0	0	0	0
4	C	12	0	0	0	0
4	D	13	0	0	0	0
4	E	13	0	0	0	0
4	F	7	0	0	0	0
4	G	7	0	0	0	0
4	H	7	0	0	0	0
All	All	17790	0	17768	99	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 3.

All (99) 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:B:262:ASN:HD21	2:L:15:GLU:CB	2.01	0.73
1:F:226:THR:HG22	1:F:227:PRO:HD2	1.72	0.72
1:F:41:ILE:HG13	1:F:42:ALA:H	1.55	0.72
1:B:20:GLU:HG2	2:T:45:GLU:HG2	1.73	0.71
1:A:262:ASN:HD21	2:K:15:GLU:CB	2.07	0.68
1:B:201:MET:HE2	1:B:220:ALA:HB1	1.77	0.66
1:A:201:MET:HE2	1:A:220:ALA:HB1	1.77	0.66
1:C:132:MET:HE3	1:F:40:ASN:HB2	1.81	0.63
1:F:41:ILE:HG13	1:F:42:ALA:N	2.14	0.62
1:A:65:ILE:O	1:A:98:ARG:NH2	2.33	0.62
1:C:65:ILE:O	1:C:98:ARG:NH2	2.32	0.62
1:F:65:ILE:O	1:F:98:ARG:NH2	2.32	0.62
1:D:65:ILE:O	1:D:98:ARG:NH2	2.33	0.61
1:E:65:ILE:O	1:E:98:ARG:NH2	2.33	0.61
1:G:65:ILE:O	1:G:98:ARG:NH2	2.33	0.60
1:H:65:ILE:O	1:H:98:ARG:NH1	2.33	0.60
1:B:65:ILE:O	1:B:98:ARG:NH2	2.33	0.59
1:H:268:GLU:HG2	1:H:269:GLY:H	1.68	0.57
1:H:142:LEU:HD21	1:H:170:LEU:HD12	1.87	0.57
1:B:166:ALA:HB2	1:E:152:VAL:HG21	1.87	0.56
1:D:142:LEU:HD21	1:D:170:LEU:HD12	1.85	0.56
1:G:201:MET:HE2	1:G:220:ALA:HB1	1.86	0.56
1:E:142:LEU:HD13	1:E:167:PHE:CD1	2.40	0.56
1:H:142:LEU:HD13	1:H:167:PHE:CD1	2.40	0.55
1:H:268:GLU:HG2	1:H:269:GLY:N	2.21	0.55
1:D:142:LEU:HD13	1:D:167:PHE:CD1	2.42	0.55
1:E:142:LEU:HD21	1:E:170:LEU:HD12	1.87	0.54
1:D:240:MET:HG3	1:D:261:VAL:HG11	1.90	0.53
1:E:240:MET:HG3	1:E:261:VAL:HG11	1.91	0.53
1:G:262:ASN:HD21	2:Q:15:GLU:CB	2.22	0.52
1:A:262:ASN:ND2	2:K:15:GLU:CB	2.72	0.52
1:B:166:ALA:CB	1:E:152:VAL:HG21	2.40	0.52
1:C:240:MET:HG3	1:C:261:VAL:HG11	1.91	0.51
1:A:166:ALA:CB	1:C:152:VAL:HG21	2.41	0.51
1:B:152:VAL:HG21	1:E:166:ALA:HB2	1.93	0.51
1:A:166:ALA:HB2	1:C:152:VAL:HG21	1.93	0.51
1:C:41:ILE:HG13	1:C:41:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:MET:HG3	1:F:261:VAL:HG11	1.93	0.50
1:G:240:MET:HG3	1:G:261:VAL:HG11	1.93	0.50
1:H:240:MET:HG3	1:H:261:VAL:HG11	1.93	0.50
1:E:41:ILE:O	1:E:41:ILE:HG13	2.12	0.50
1:B:167:PHE:CD1	1:B:170:LEU:HD12	2.47	0.49
1:C:36:ARG:HG2	1:F:122:SER:O	2.11	0.49
1:D:162:SER:HB3	1:F:163:VAL:CG2	2.42	0.49
1:C:201:MET:HE2	1:C:220:ALA:HB1	1.93	0.49
1:F:42:ALA:O	1:F:43:SER:CB	2.62	0.48
1:G:41:ILE:HG13	1:G:41:ILE:O	2.14	0.48
1:A:39:MET:HE3	1:D:119:PHE:HD2	1.79	0.48
1:A:201:MET:CE	1:A:220:ALA:HB1	2.42	0.47
1:B:201:MET:CE	1:B:220:ALA:HB1	2.45	0.47
1:E:118:GLY:HA2	1:G:39:MET:O	2.15	0.46
1:C:104:LEU:HB3	1:F:41:ILE:CD1	2.45	0.46
1:C:142:LEU:HD21	1:C:170:LEU:HD12	1.97	0.46
1:B:121:HIS:CE1	1:H:35:LEU:HD13	2.51	0.46
1:B:262:ASN:ND2	2:L:15:GLU:CB	2.75	0.46
1:A:240:MET:HG3	1:A:261:VAL:HG11	1.98	0.46
2:T:45:GLU:HG3	2:T:64:GLU:HB2	1.98	0.46
1:E:119:PHE:HB2	1:G:39:MET:HE3	1.97	0.46
1:B:14:SER:N	2:L:14:GLU:OE1	2.29	0.45
1:B:240:MET:HG3	1:B:261:VAL:HG11	1.98	0.45
1:D:166:ALA:HB1	1:F:167:PHE:CE1	2.52	0.45
1:C:142:LEU:HD13	1:C:167:PHE:CD2	2.52	0.45
1:A:79:GLN:O	1:A:83:MET:HG3	2.17	0.44
1:C:119:PHE:HD2	1:F:39:MET:HE3	1.83	0.44
1:C:39:MET:HE3	1:F:119:PHE:HD2	1.82	0.44
1:G:201:MET:CE	1:G:220:ALA:HB1	2.47	0.44
1:B:16:ARG:O	1:B:20:GLU:HG3	2.17	0.44
1:B:167:PHE:CE1	1:B:170:LEU:HD12	2.53	0.43
1:B:39:MET:HE3	1:H:119:PHE:HD2	1.83	0.43
1:C:41:ILE:HD13	1:F:104:LEU:HB3	1.99	0.43
1:F:42:ALA:O	1:F:43:SER:HB3	2.18	0.43
1:C:187:ASP:OD1	1:C:203:ARG:HB2	2.19	0.43
1:B:119:PHE:HD2	1:H:39:MET:HE3	1.84	0.43
1:B:187:ASP:OD1	1:B:203:ARG:HB2	2.19	0.43
1:C:201:MET:CE	1:C:220:ALA:HB1	2.49	0.43
1:B:39:MET:O	1:H:118:GLY:HA2	2.19	0.42
1:D:187:ASP:OD1	1:D:203:ARG:HB2	2.19	0.42
1:E:187:ASP:OD1	1:E:203:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLN:O	1:B:83:MET:HG3	2.18	0.42
1:H:187:ASP:OD1	1:H:203:ARG:HB2	2.18	0.42
1:A:119:PHE:HD2	1:D:39:MET:HE3	1.84	0.42
1:F:262:ASN:HD21	2:P:15:GLU:CB	2.31	0.42
1:A:223:ILE:HD12	4:A:525:HOH:O	2.19	0.42
1:C:119:PHE:CE2	1:F:41:ILE:HG21	2.54	0.42
1:G:79:GLN:O	1:G:83:MET:HG3	2.19	0.42
1:F:187:ASP:OD1	1:F:203:ARG:HB2	2.19	0.42
1:B:20:GLU:CG	2:T:45:GLU:HG2	2.46	0.42
1:E:201:MET:HE2	1:E:220:ALA:HB1	2.02	0.42
1:C:118:GLY:HA2	1:F:39:MET:O	2.20	0.41
1:A:187:ASP:OD1	1:A:203:ARG:HB2	2.20	0.41
1:D:152:VAL:HG11	1:D:163:VAL:HG11	2.03	0.41
1:F:133:VAL:HG21	1:F:176:VAL:HG12	2.03	0.41
1:G:133:VAL:HG21	1:G:176:VAL:HG12	2.03	0.41
1:A:133:VAL:HG21	1:A:176:VAL:HG12	2.03	0.41
1:G:187:ASP:OD1	1:G:203:ARG:HB2	2.19	0.41
1:H:152:VAL:HG11	1:H:163:VAL:HG11	2.02	0.41
1:F:139:VAL:HG21	3:F:401:ADP:C6	2.56	0.40
1:B:133:VAL:HG21	1:B:176:VAL:HG12	2.04	0.40
1:B:166:ALA:HB2	1:E:152:VAL:CG2	2.52	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	290/314 (92%)	283 (98%)	7 (2%)	0	100	100
1	B	283/314 (90%)	276 (98%)	7 (2%)	0	100	100
1	C	280/314 (89%)	274 (98%)	6 (2%)	0	100	100
1	D	291/314 (93%)	284 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	288/314 (92%)	282 (98%)	6 (2%)	0	100 100
1	F	273/314 (87%)	266 (97%)	6 (2%)	1 (0%)	34 48
1	G	282/314 (90%)	276 (98%)	6 (2%)	0	100 100
1	H	275/314 (88%)	270 (98%)	5 (2%)	0	100 100
2	K	3/60 (5%)	2 (67%)	1 (33%)	0	100 100
2	L	3/60 (5%)	3 (100%)	0	0	100 100
2	M	3/60 (5%)	0	2 (67%)	1 (33%)	0 0
2	N	1/60 (2%)	0	1 (100%)	0	100 100
2	O	1/60 (2%)	0	1 (100%)	0	100 100
2	P	3/60 (5%)	2 (67%)	1 (33%)	0	100 100
2	Q	3/60 (5%)	1 (33%)	2 (67%)	0	100 100
2	T	20/60 (33%)	18 (90%)	2 (10%)	0	100 100
All	All	2299/2992 (77%)	2237 (97%)	60 (3%)	2 (0%)	51 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	43	SER
2	M	14	GLU

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	229/252 (91%)	225 (98%)	4 (2%)	60 78
1	B	225/252 (89%)	221 (98%)	4 (2%)	59 76
1	C	223/252 (88%)	219 (98%)	4 (2%)	59 76
1	D	227/252 (90%)	225 (99%)	2 (1%)	78 90
1	E	225/252 (89%)	221 (98%)	4 (2%)	59 76
1	F	219/252 (87%)	215 (98%)	4 (2%)	59 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	221/252 (88%)	217 (98%)	4 (2%)	59 76
1	H	218/252 (86%)	213 (98%)	5 (2%)	50 70
2	K	3/60 (5%)	3 (100%)	0	100 100
2	L	3/60 (5%)	3 (100%)	0	100 100
2	M	3/60 (5%)	3 (100%)	0	100 100
2	N	2/60 (3%)	2 (100%)	0	100 100
2	O	2/60 (3%)	2 (100%)	0	100 100
2	P	3/60 (5%)	3 (100%)	0	100 100
2	Q	3/60 (5%)	2 (67%)	1 (33%)	0 0
2	T	20/60 (33%)	18 (90%)	2 (10%)	7 11
All	All	1826/2496 (73%)	1792 (98%)	34 (2%)	57 75

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	56	GLU
1	A	157	GLU
1	A	200	SER
1	B	40	ASN
1	B	142	LEU
1	B	168	MET
1	B	200	SER
1	C	157	GLU
1	C	172	HIS
1	C	195	ASP
1	C	200	SER
1	D	172	HIS
1	D	200	SER
1	E	11	ARG
1	E	157	GLU
1	E	172	HIS
1	E	200	SER
1	F	157	GLU
1	F	168	MET
1	F	200	SER
1	F	226	THR
1	G	40	ASN

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Mol	Chain	Res	Type
1	G	157	GLU
1	G	168	MET
1	G	200	SER
1	H	45	LYS
1	H	91	SER
1	H	157	GLU
1	H	172	HIS
1	H	200	SER
2	Q	12	GLU
2	T	23	GLU
2	T	47	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	47	GLN
1	A	253	ASN
1	B	40	ASN
1	B	47	GLN
1	B	253	ASN
1	B	262	ASN
1	C	253	ASN
1	D	253	ASN
1	E	253	ASN
1	F	253	ASN
1	G	253	ASN
1	H	253	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	ADP	G	401	-	18,21,29	0.61	0	18,31,45	0.93	2 (11%)
3	ADP	E	401	-	18,21,29	0.65	0	18,31,45	0.96	1 (5%)
3	ADP	H	401	-	18,21,29	0.59	0	18,31,45	0.91	2 (11%)
3	ADP	C	401	-	18,21,29	0.63	0	18,31,45	0.72	1 (5%)
3	ADP	B	401	-	18,21,29	0.64	0	18,31,45	0.80	1 (5%)
3	ADP	F	401	-	18,21,29	0.64	0	18,31,45	0.74	1 (5%)
3	ADP	D	401	-	18,21,29	0.64	0	18,31,45	0.72	1 (5%)
3	ADP	A	401	-	18,21,29	0.64	0	18,31,45	0.85	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	ADP	G	401	-	-	0/2/22/32	0/3/3/3
3	ADP	E	401	-	-	2/2/22/32	0/3/3/3
3	ADP	H	401	-	-	2/2/22/32	0/3/3/3
3	ADP	C	401	-	-	0/2/22/32	0/3/3/3
3	ADP	B	401	-	-	2/2/22/32	0/3/3/3
3	ADP	F	401	-	-	0/2/22/32	0/3/3/3
3	ADP	D	401	-	-	0/2/22/32	0/3/3/3
3	ADP	A	401	-	-	2/2/22/32	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	401	ADP	C3'-C2'-C1'	2.54	104.81	100.98
3	G	401	ADP	C3'-C2'-C1'	2.43	104.63	100.98
3	H	401	ADP	C5-C6-N6	2.28	123.82	120.35
3	F	401	ADP	C5-C6-N6	2.21	123.71	120.35
3	C	401	ADP	C5-C6-N6	2.14	123.60	120.35
3	D	401	ADP	C5-C6-N6	2.10	123.55	120.35
3	H	401	ADP	C3'-C2'-C1'	2.08	104.11	100.98
3	G	401	ADP	C5-C6-N6	2.03	123.44	120.35
3	B	401	ADP	C5-C6-N6	2.00	123.40	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

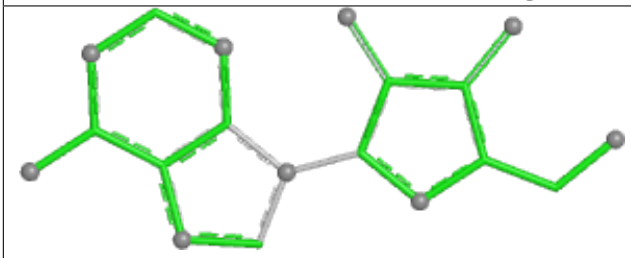
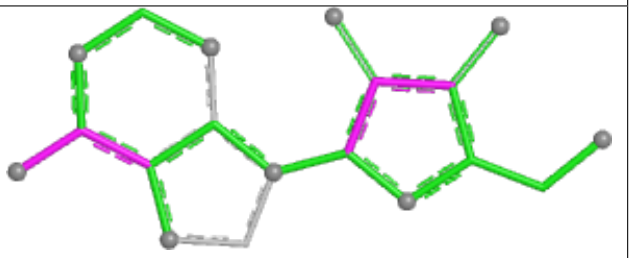
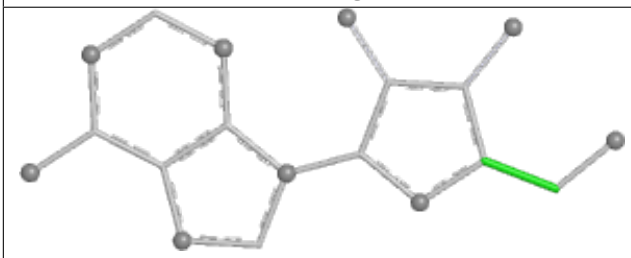
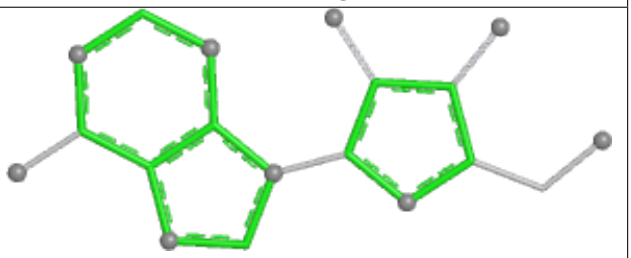
Mol	Chain	Res	Type	Atoms
3	A	401	ADP	O4'-C4'-C5'-O5'
3	E	401	ADP	O4'-C4'-C5'-O5'
3	H	401	ADP	O4'-C4'-C5'-O5'
3	A	401	ADP	C3'-C4'-C5'-O5'
3	H	401	ADP	C3'-C4'-C5'-O5'
3	E	401	ADP	C3'-C4'-C5'-O5'
3	B	401	ADP	O4'-C4'-C5'-O5'
3	B	401	ADP	C3'-C4'-C5'-O5'

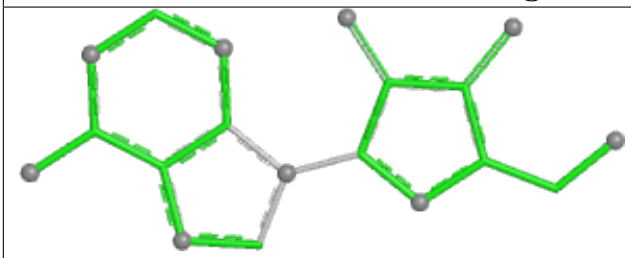
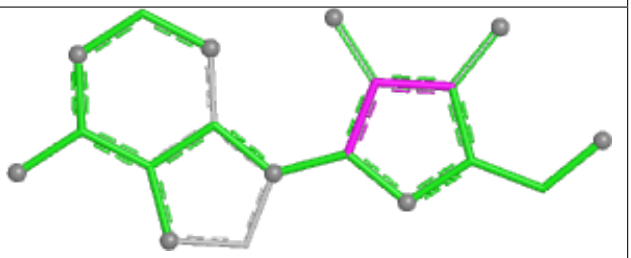
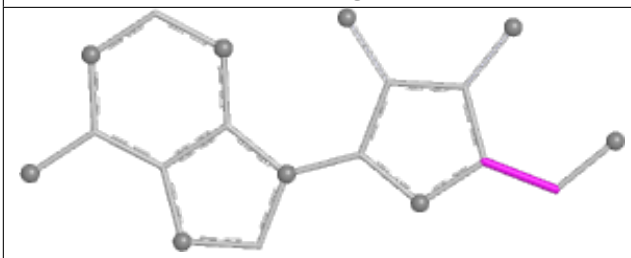
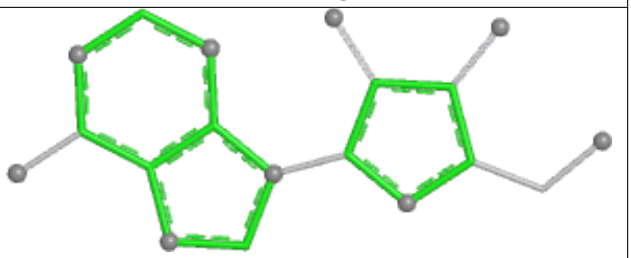
There are no ring outliers.

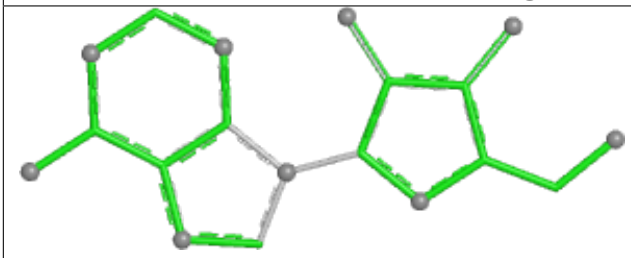
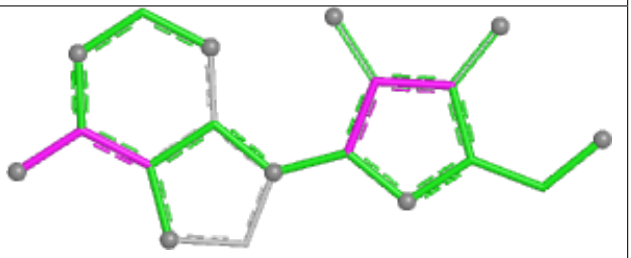
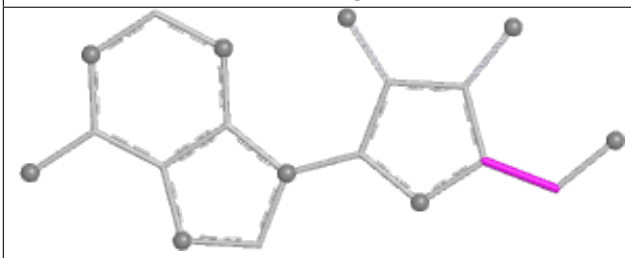
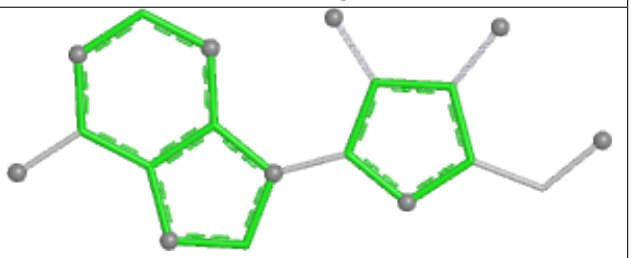
1 monomer is involved in 1 short contact:

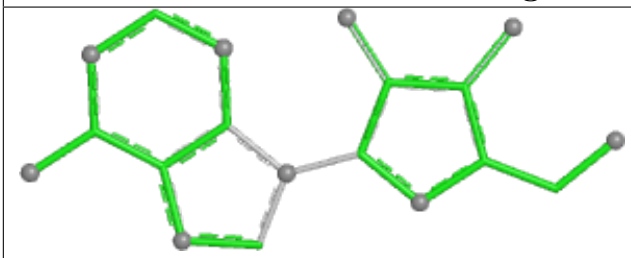
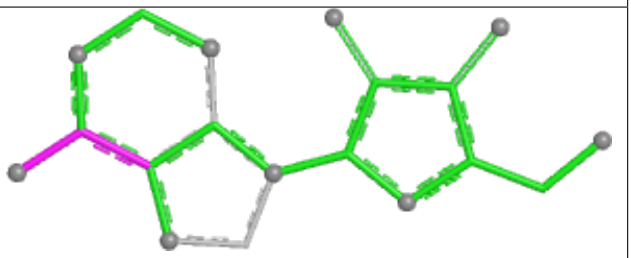
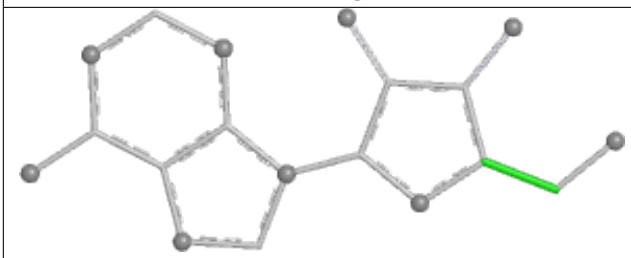
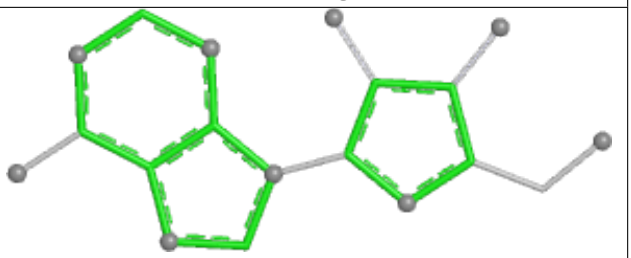
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	ADP	1	0

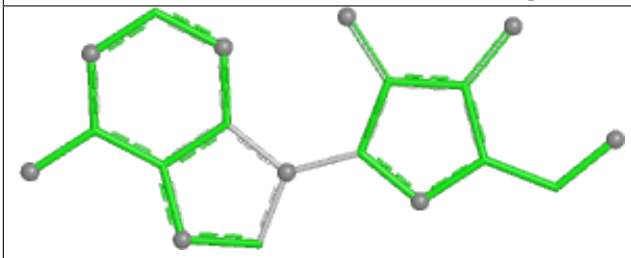
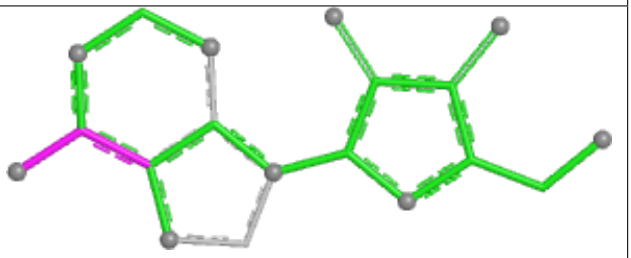
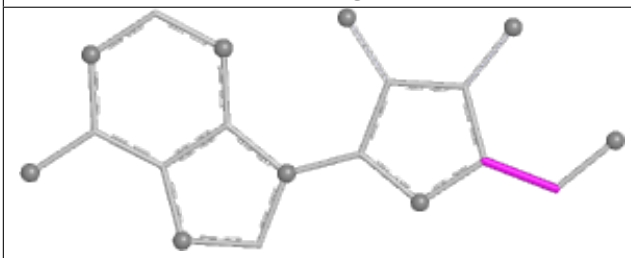
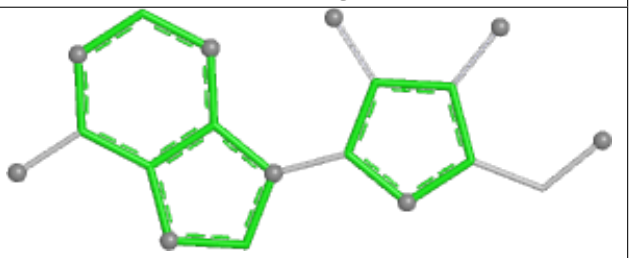
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

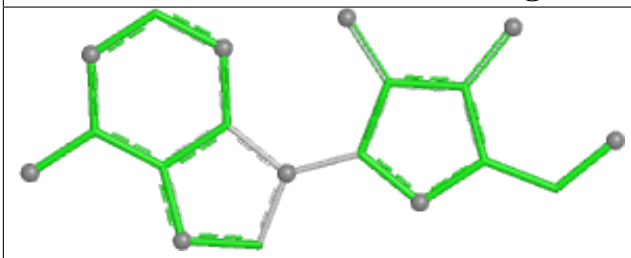
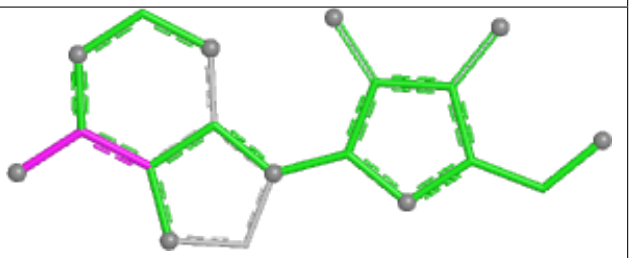
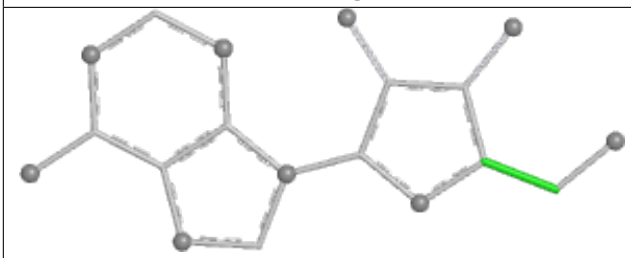
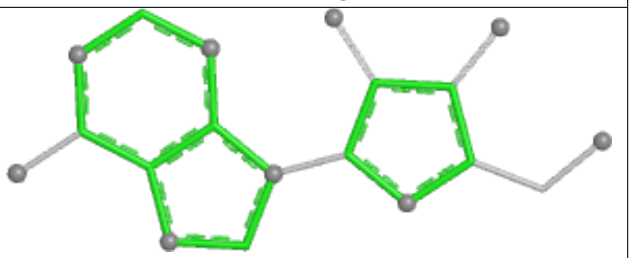
Ligand ADP G 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

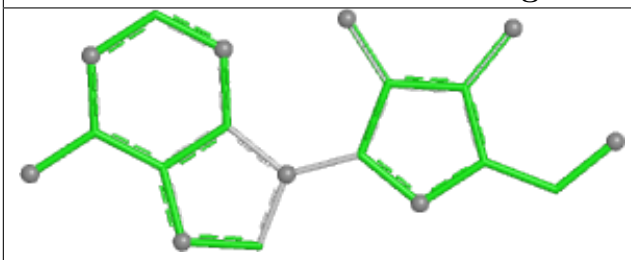
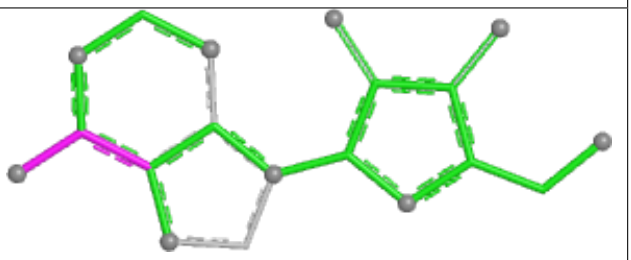
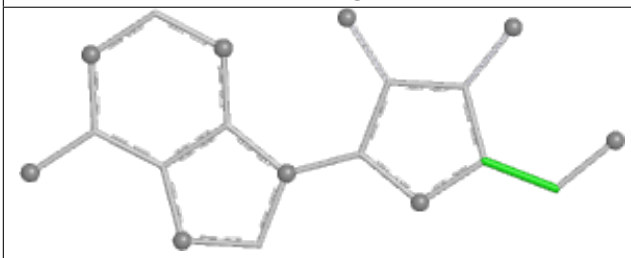
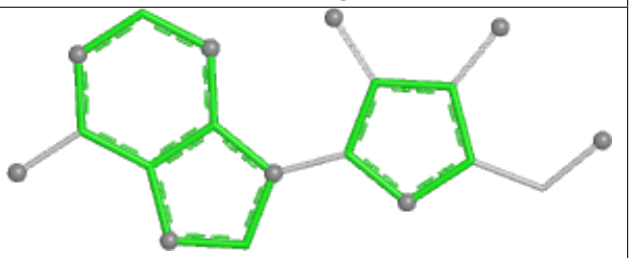
Ligand ADP E 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

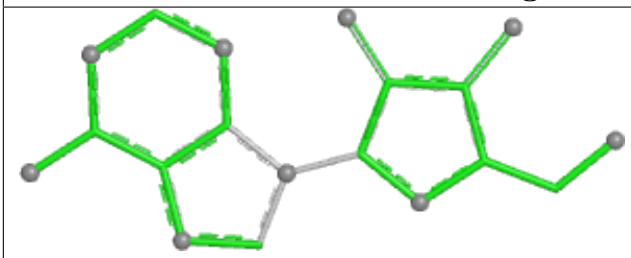
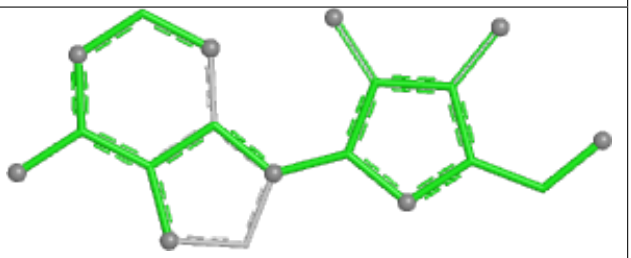
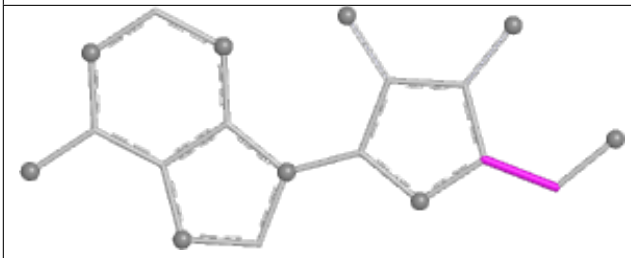
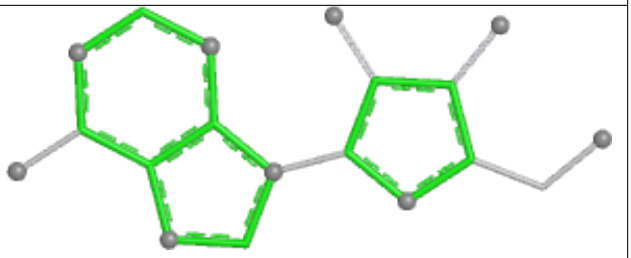
Ligand ADP H 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP F 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	T	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	33:GLU	C	41:GLU	N	21.13
1	T	47:GLU	C	61:GLU	N	19.51

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	292/314 (92%)	0.41	5 (1%) 70 68	45, 60, 89, 139	0
1	B	287/314 (91%)	0.34	2 (0%) 87 86	49, 69, 99, 129	0
1	C	284/314 (90%)	0.47	7 (2%) 57 55	48, 68, 99, 121	0
1	D	293/314 (93%)	0.68	18 (6%) 21 20	46, 73, 107, 145	0
1	E	290/314 (92%)	0.37	1 (0%) 94 93	51, 70, 105, 122	0
1	F	277/314 (88%)	0.74	28 (10%) 7 6	52, 86, 120, 144	0
1	G	286/314 (91%)	0.69	24 (8%) 11 10	61, 86, 122, 169	0
1	H	279/314 (88%)	0.56	20 (7%) 15 14	49, 75, 108, 118	0
2	K	5/60 (8%)	0.06	0 100 100	90, 93, 99, 101	0
2	L	5/60 (8%)	1.85	1 (20%) 1 0	110, 114, 122, 130	0
2	M	5/60 (8%)	2.60	2 (40%) 0 0	111, 111, 125, 126	0
2	N	3/60 (5%)	2.08	2 (66%) 0 0	133, 133, 134, 136	0
2	O	3/60 (5%)	1.92	2 (66%) 0 0	112, 112, 113, 117	0
2	P	5/60 (8%)	1.04	1 (20%) 1 0	118, 125, 128, 131	0
2	Q	5/60 (8%)	2.03	2 (40%) 0 0	112, 114, 115, 124	0
2	T	26/60 (43%)	1.42	9 (34%) 0 0	78, 101, 147, 150	0
All	All	2345/2992 (78%)	0.56	124 (5%) 26 25	45, 73, 115, 169	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	11	GLU	7.4
1	F	250	LEU	5.6
2	Q	15	GLU	5.3
1	F	45	LYS	5.0
1	D	206	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	47	GLN	4.8
1	F	188	ILE	4.7
2	T	26	GLU	4.6
1	G	207	PRO	4.6
1	F	44	HIS	4.6
1	D	292	PRO	4.5
1	F	258	VAL	4.5
1	G	183	ALA	4.4
2	L	11	GLU	4.3
2	T	25	GLU	4.2
1	F	43	SER	4.1
1	B	217	GLY	4.1
1	F	42	ALA	3.9
1	D	210	PHE	3.9
1	G	210	PHE	3.9
1	H	52	GLY	3.9
1	F	249	ILE	3.8
1	G	212	SER	3.7
1	H	1	MET	3.7
1	A	206	ALA	3.6
1	G	186	ALA	3.4
1	F	51	ARG	3.4
1	H	85	VAL	3.3
1	D	208	GLY	3.3
2	T	24	GLU	3.2
2	T	22	GLU	3.2
1	H	51	ARG	3.2
2	T	42	GLU	3.1
1	G	250	LEU	3.1
1	H	38	TYR	3.1
2	N	14	GLU	3.0
1	D	212	SER	3.0
1	C	52	GLY	3.0
1	D	224	LYS	3.0
2	T	28	GLU	2.9
1	D	215	HIS	2.9
1	G	119	PHE	2.9
2	T	21	GLU	2.9
1	A	210	PHE	2.9
1	B	210	PHE	2.8
1	H	57	GLY	2.8
1	F	203	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	211	ARG	2.8
1	F	195	ASP	2.7
1	F	119	PHE	2.7
1	H	56	GLU	2.7
2	P	11	GLU	2.7
1	A	214	LEU	2.7
1	G	154	CYS	2.6
1	G	219	SER	2.6
1	H	54	PRO	2.6
1	H	50	TYR	2.6
1	C	42	ALA	2.6
1	H	46	PRO	2.6
1	H	207	PRO	2.6
1	G	106	LEU	2.5
1	D	189	ARG	2.5
1	F	256	PRO	2.5
1	H	19	VAL	2.5
1	F	187	ASP	2.5
1	G	249	ILE	2.5
1	H	2	LYS	2.5
1	C	53	GLN	2.5
1	G	47	GLN	2.5
1	D	207	PRO	2.5
1	H	26	GLY	2.5
2	T	29	GLU	2.5
1	F	232	THR	2.5
1	G	206	ALA	2.5
1	H	55	LEU	2.5
1	H	80	PHE	2.5
1	G	251	ARG	2.4
1	F	270	ILE	2.4
1	H	195	ASP	2.4
1	C	119	PHE	2.4
2	T	23	GLU	2.4
1	A	212	SER	2.4
1	G	138	LEU	2.4
1	G	184	GLY	2.4
2	M	12	GLU	2.4
1	A	207	PRO	2.3
1	F	257	LEU	2.3
1	G	262	ASN	2.3
1	F	254	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	259	MET	2.3
1	F	184	GLY	2.3
1	F	200	SER	2.3
1	C	212	SER	2.3
1	D	219	SER	2.2
1	G	195	ASP	2.2
1	G	188	ILE	2.2
1	G	220	ALA	2.2
1	D	179	TYR	2.2
1	F	247	VAL	2.2
1	D	57	GLY	2.2
2	Q	11	GLU	2.2
1	D	176	VAL	2.1
1	E	32	ILE	2.1
1	H	290	GLY	2.1
1	C	207	PRO	2.1
1	F	238	ARG	2.1
1	G	133	VAL	2.1
2	O	14	GLU	2.1
1	F	3	ILE	2.1
1	D	138	LEU	2.1
1	G	187	ASP	2.1
1	D	142	LEU	2.1
1	C	142	LEU	2.1
1	F	236	ALA	2.1
1	D	153	LEU	2.1
1	H	58	PHE	2.1
1	H	9	ASN	2.1
1	G	255	GLY	2.1
1	D	143	LEU	2.1
1	D	291	GLY	2.1
2	O	13	GLU	2.0
1	F	104	LEU	2.0
1	F	278	ILE	2.0
2	N	13	GLU	2.0

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)

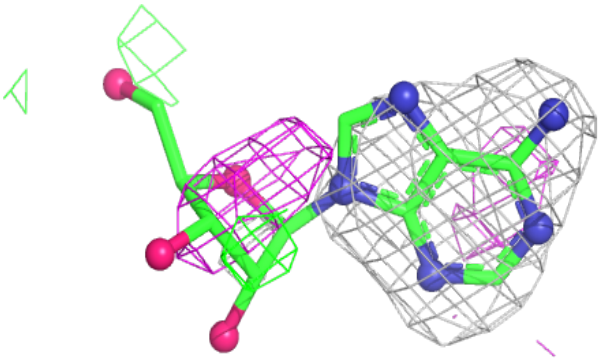
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

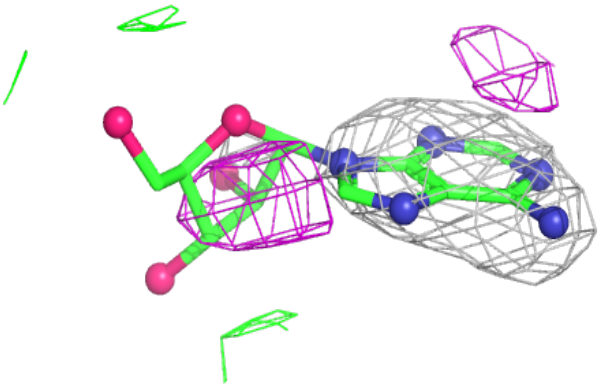
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	D	401	19/27	0.70	0.59	87,117,160,162	0
3	ADP	H	401	19/27	0.74	0.34	78,103,137,137	0
3	ADP	G	401	19/27	0.81	0.45	85,101,139,142	0
3	ADP	F	401	19/27	0.82	0.39	89,105,146,148	0
3	ADP	E	401	19/27	0.83	0.32	61,75,103,103	0
3	ADP	C	401	19/27	0.84	0.29	58,77,125,129	0
3	ADP	A	401	19/27	0.89	0.29	49,67,105,105	0
3	ADP	B	401	19/27	0.92	0.28	58,75,118,120	0

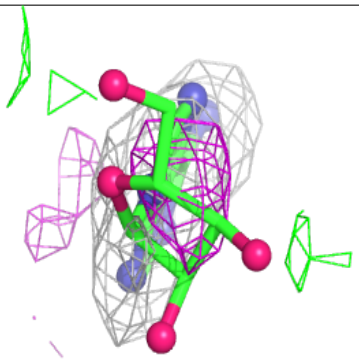
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 401:

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

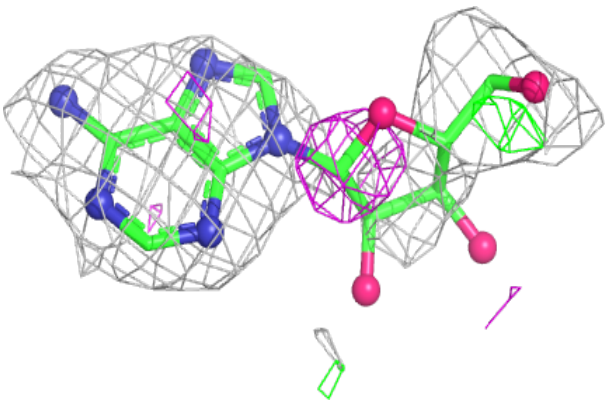


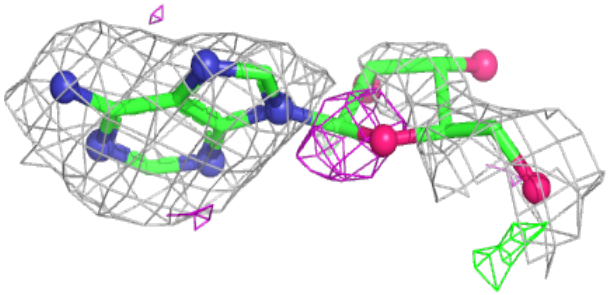


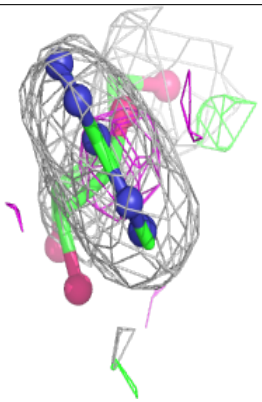


Electron density around ADP H 401:

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

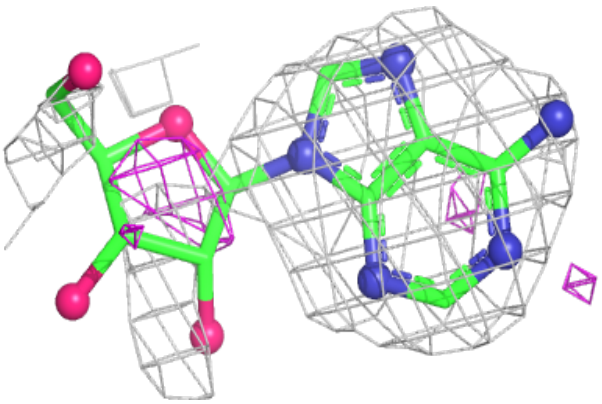


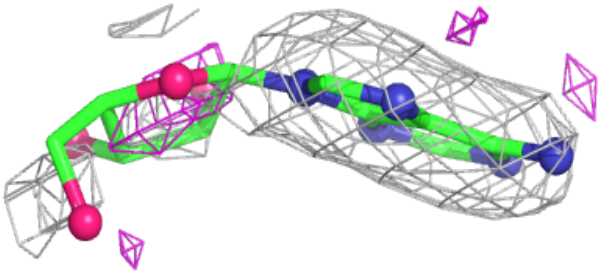


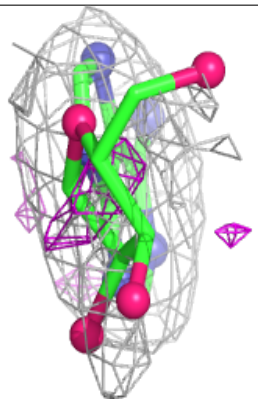


Electron density around ADP G 401:

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

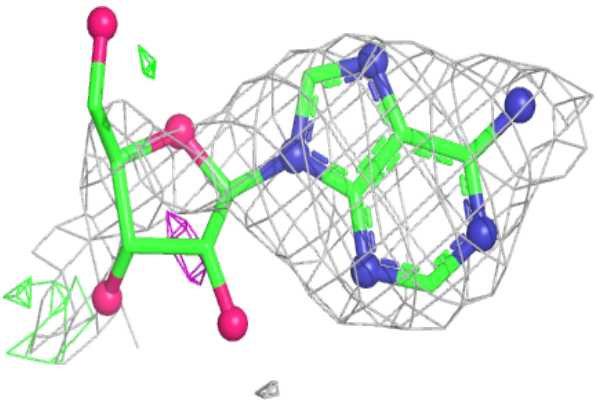


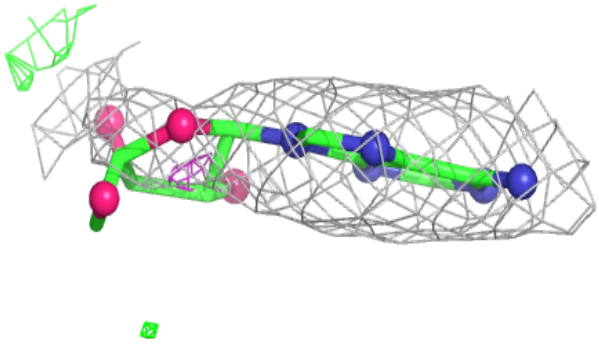


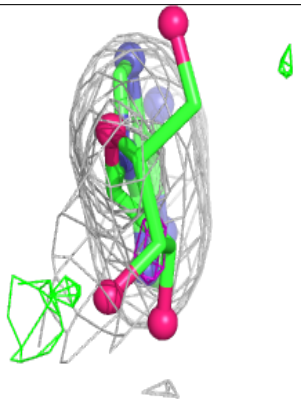


Electron density around ADP F 401:

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

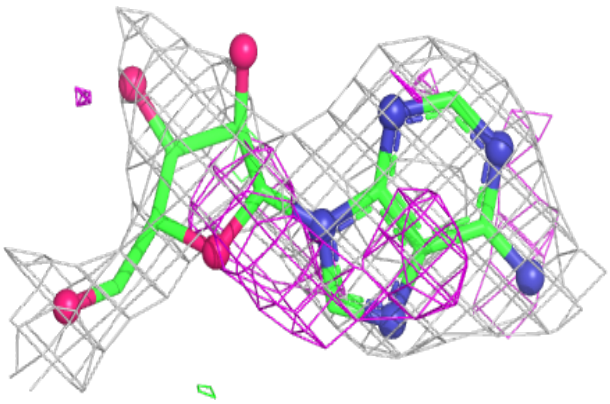


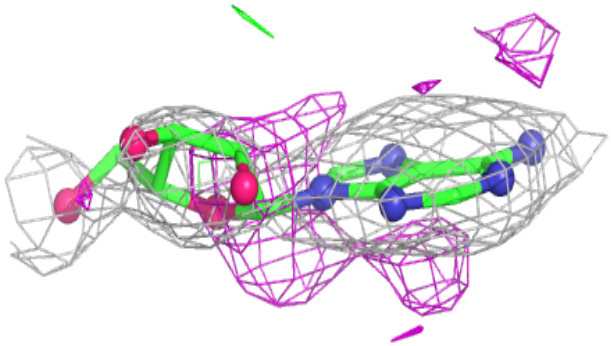


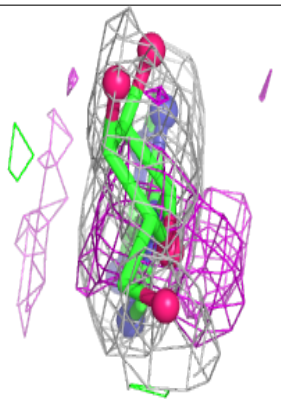


Electron density around ADP E 401:

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

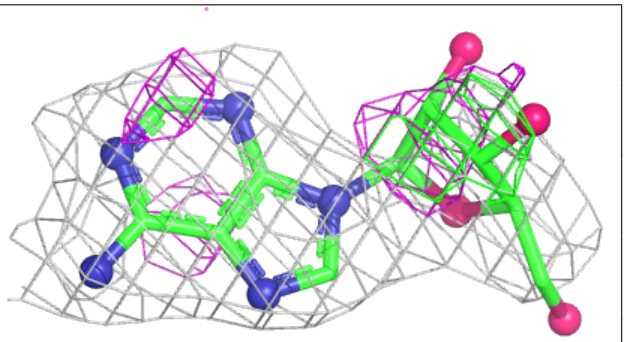


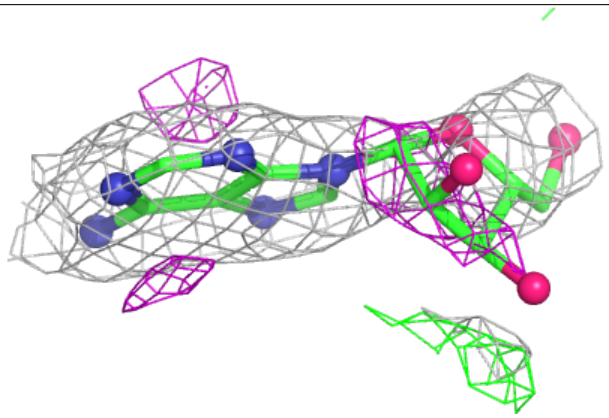


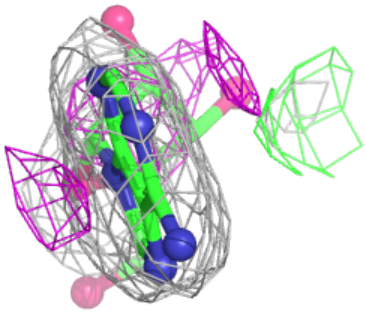


Electron density around ADP C 401:

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

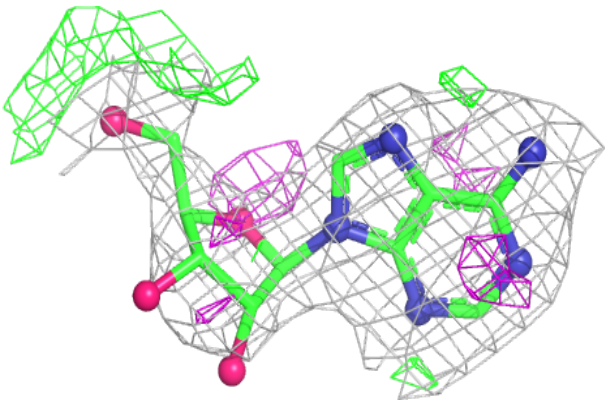


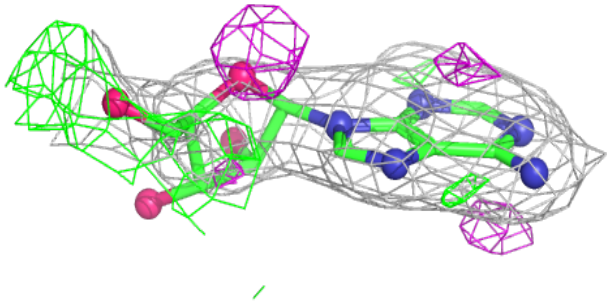


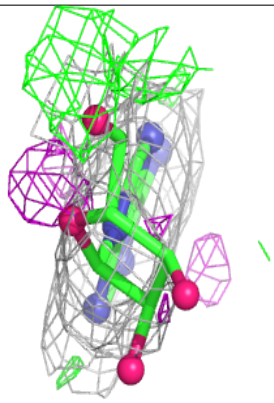


Electron density around ADP A 401:

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

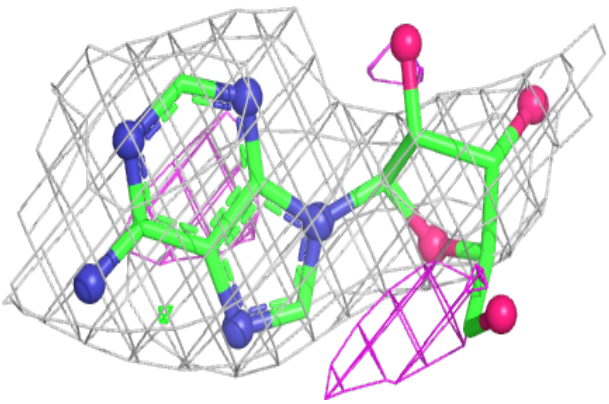


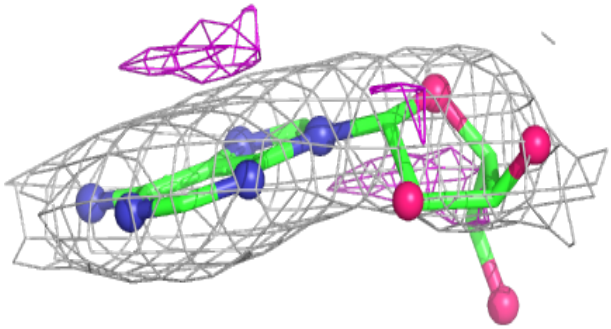


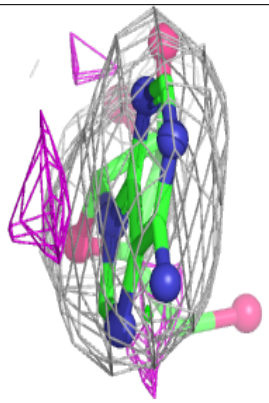


Electron density around ADP B 401:

$2mF_o$-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.