



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:25 AM BST

PDB ID : 5DM3
Title : Crystal Structure of Glutamine Synthetase from *Chromohalobacter salexigens* DSM 3043(Csal_0679, TARGET EFI-550015) with bound ADP
Authors : Yadava, U.; Vetting, M.W.; Al Obaidi, N.F.; Toro, R.; Morisco, L.L.; Benach, J.; Koss, J.; Wasserman, S.R.; Attonito, J.D.; Scott Glenn, A.; Chamala, S.; Chowdhury, S.; Lafleur, J.; Love, J.; Seidel, R.D.; Whalen, K.L.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2015-09-07
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

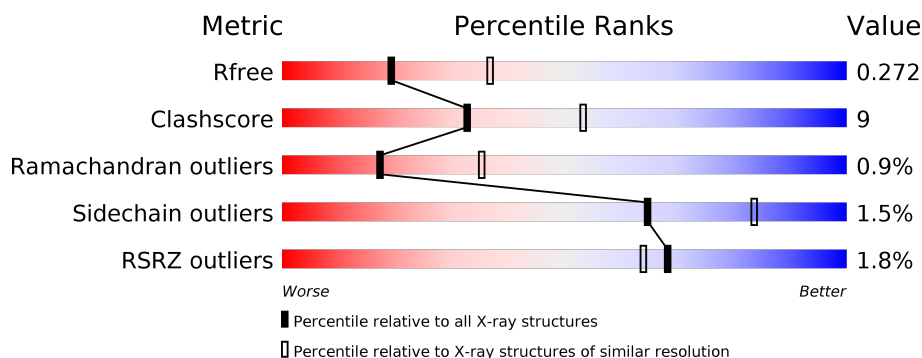
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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 $\leq 5\%$. 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	475	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>15%</div> <div>•</div> <div>21%</div> </div> </div>
1	B	475	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>21%</div> <div>•</div> <div>19%</div> </div> </div>
1	C	475	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div></div> <div>17%</div> </div> </div>
1	D	475	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>16%</div> <div>•</div> <div>19%</div> </div> </div>
1	E	475	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>•</div> <div>19%</div> </div> </div>
1	F	475	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>18%</div> <div>•</div> <div>20%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17834 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 L-glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2859	1812	509	518	20			
1	B	385	Total	C	N	O	S	0	0	0
			2960	1871	525	543	21			
1	C	396	Total	C	N	O	S	0	1	0
			3014	1912	532	549	21			
1	D	386	Total	C	N	O	S	0	0	0
			2964	1876	527	540	21			
1	E	383	Total	C	N	O	S	0	0	0
			2925	1857	509	539	20			
1	F	381	Total	C	N	O	S	0	0	0
			2890	1837	507	525	21			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q1QZR8
A	-20	HIS	-	expression tag	UNP Q1QZR8
A	-19	HIS	-	expression tag	UNP Q1QZR8
A	-18	HIS	-	expression tag	UNP Q1QZR8
A	-17	HIS	-	expression tag	UNP Q1QZR8
A	-16	HIS	-	expression tag	UNP Q1QZR8
A	-15	HIS	-	expression tag	UNP Q1QZR8
A	-14	SER	-	expression tag	UNP Q1QZR8
A	-13	SER	-	expression tag	UNP Q1QZR8
A	-12	GLY	-	expression tag	UNP Q1QZR8
A	-11	VAL	-	expression tag	UNP Q1QZR8
A	-10	ASP	-	expression tag	UNP Q1QZR8
A	-9	LEU	-	expression tag	UNP Q1QZR8
A	-8	GLY	-	expression tag	UNP Q1QZR8
A	-7	THR	-	expression tag	UNP Q1QZR8
A	-6	GLU	-	expression tag	UNP Q1QZR8
A	-5	ASN	-	expression tag	UNP Q1QZR8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LEU	-	expression tag	UNP Q1QZR8
A	-3	TYR	-	expression tag	UNP Q1QZR8
A	-2	PHE	-	expression tag	UNP Q1QZR8
A	-1	GLN	-	expression tag	UNP Q1QZR8
A	0	SER	-	expression tag	UNP Q1QZR8
B	-21	MET	-	initiating methionine	UNP Q1QZR8
B	-20	HIS	-	expression tag	UNP Q1QZR8
B	-19	HIS	-	expression tag	UNP Q1QZR8
B	-18	HIS	-	expression tag	UNP Q1QZR8
B	-17	HIS	-	expression tag	UNP Q1QZR8
B	-16	HIS	-	expression tag	UNP Q1QZR8
B	-15	HIS	-	expression tag	UNP Q1QZR8
B	-14	SER	-	expression tag	UNP Q1QZR8
B	-13	SER	-	expression tag	UNP Q1QZR8
B	-12	GLY	-	expression tag	UNP Q1QZR8
B	-11	VAL	-	expression tag	UNP Q1QZR8
B	-10	ASP	-	expression tag	UNP Q1QZR8
B	-9	LEU	-	expression tag	UNP Q1QZR8
B	-8	GLY	-	expression tag	UNP Q1QZR8
B	-7	THR	-	expression tag	UNP Q1QZR8
B	-6	GLU	-	expression tag	UNP Q1QZR8
B	-5	ASN	-	expression tag	UNP Q1QZR8
B	-4	LEU	-	expression tag	UNP Q1QZR8
B	-3	TYR	-	expression tag	UNP Q1QZR8
B	-2	PHE	-	expression tag	UNP Q1QZR8
B	-1	GLN	-	expression tag	UNP Q1QZR8
B	0	SER	-	expression tag	UNP Q1QZR8
C	-21	MET	-	initiating methionine	UNP Q1QZR8
C	-20	HIS	-	expression tag	UNP Q1QZR8
C	-19	HIS	-	expression tag	UNP Q1QZR8
C	-18	HIS	-	expression tag	UNP Q1QZR8
C	-17	HIS	-	expression tag	UNP Q1QZR8
C	-16	HIS	-	expression tag	UNP Q1QZR8
C	-15	HIS	-	expression tag	UNP Q1QZR8
C	-14	SER	-	expression tag	UNP Q1QZR8
C	-13	SER	-	expression tag	UNP Q1QZR8
C	-12	GLY	-	expression tag	UNP Q1QZR8
C	-11	VAL	-	expression tag	UNP Q1QZR8
C	-10	ASP	-	expression tag	UNP Q1QZR8
C	-9	LEU	-	expression tag	UNP Q1QZR8
C	-8	GLY	-	expression tag	UNP Q1QZR8
C	-7	THR	-	expression tag	UNP Q1QZR8

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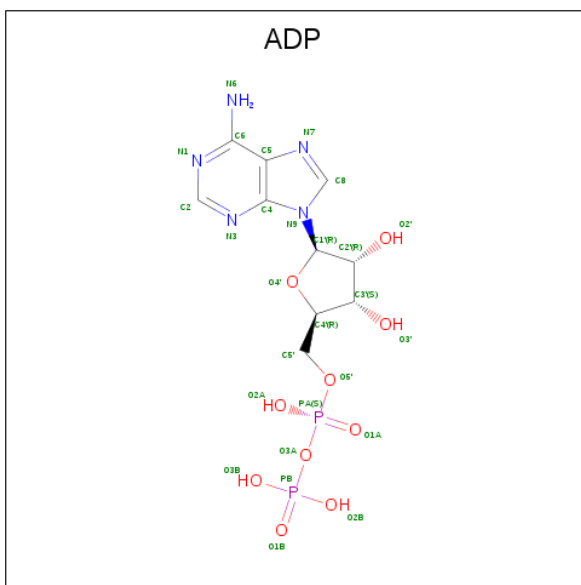
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLU	-	expression tag	UNP Q1QZR8
C	-5	ASN	-	expression tag	UNP Q1QZR8
C	-4	LEU	-	expression tag	UNP Q1QZR8
C	-3	TYR	-	expression tag	UNP Q1QZR8
C	-2	PHE	-	expression tag	UNP Q1QZR8
C	-1	GLN	-	expression tag	UNP Q1QZR8
C	0	SER	-	expression tag	UNP Q1QZR8
D	-21	MET	-	initiating methionine	UNP Q1QZR8
D	-20	HIS	-	expression tag	UNP Q1QZR8
D	-19	HIS	-	expression tag	UNP Q1QZR8
D	-18	HIS	-	expression tag	UNP Q1QZR8
D	-17	HIS	-	expression tag	UNP Q1QZR8
D	-16	HIS	-	expression tag	UNP Q1QZR8
D	-15	HIS	-	expression tag	UNP Q1QZR8
D	-14	SER	-	expression tag	UNP Q1QZR8
D	-13	SER	-	expression tag	UNP Q1QZR8
D	-12	GLY	-	expression tag	UNP Q1QZR8
D	-11	VAL	-	expression tag	UNP Q1QZR8
D	-10	ASP	-	expression tag	UNP Q1QZR8
D	-9	LEU	-	expression tag	UNP Q1QZR8
D	-8	GLY	-	expression tag	UNP Q1QZR8
D	-7	THR	-	expression tag	UNP Q1QZR8
D	-6	GLU	-	expression tag	UNP Q1QZR8
D	-5	ASN	-	expression tag	UNP Q1QZR8
D	-4	LEU	-	expression tag	UNP Q1QZR8
D	-3	TYR	-	expression tag	UNP Q1QZR8
D	-2	PHE	-	expression tag	UNP Q1QZR8
D	-1	GLN	-	expression tag	UNP Q1QZR8
D	0	SER	-	expression tag	UNP Q1QZR8
E	-21	MET	-	initiating methionine	UNP Q1QZR8
E	-20	HIS	-	expression tag	UNP Q1QZR8
E	-19	HIS	-	expression tag	UNP Q1QZR8
E	-18	HIS	-	expression tag	UNP Q1QZR8
E	-17	HIS	-	expression tag	UNP Q1QZR8
E	-16	HIS	-	expression tag	UNP Q1QZR8
E	-15	HIS	-	expression tag	UNP Q1QZR8
E	-14	SER	-	expression tag	UNP Q1QZR8
E	-13	SER	-	expression tag	UNP Q1QZR8
E	-12	GLY	-	expression tag	UNP Q1QZR8
E	-11	VAL	-	expression tag	UNP Q1QZR8
E	-10	ASP	-	expression tag	UNP Q1QZR8
E	-9	LEU	-	expression tag	UNP Q1QZR8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	GLY	-	expression tag	UNP Q1QZR8
E	-7	THR	-	expression tag	UNP Q1QZR8
E	-6	GLU	-	expression tag	UNP Q1QZR8
E	-5	ASN	-	expression tag	UNP Q1QZR8
E	-4	LEU	-	expression tag	UNP Q1QZR8
E	-3	TYR	-	expression tag	UNP Q1QZR8
E	-2	PHE	-	expression tag	UNP Q1QZR8
E	-1	GLN	-	expression tag	UNP Q1QZR8
E	0	SER	-	expression tag	UNP Q1QZR8
F	-21	MET	-	initiating methionine	UNP Q1QZR8
F	-20	HIS	-	expression tag	UNP Q1QZR8
F	-19	HIS	-	expression tag	UNP Q1QZR8
F	-18	HIS	-	expression tag	UNP Q1QZR8
F	-17	HIS	-	expression tag	UNP Q1QZR8
F	-16	HIS	-	expression tag	UNP Q1QZR8
F	-15	HIS	-	expression tag	UNP Q1QZR8
F	-14	SER	-	expression tag	UNP Q1QZR8
F	-13	SER	-	expression tag	UNP Q1QZR8
F	-12	GLY	-	expression tag	UNP Q1QZR8
F	-11	VAL	-	expression tag	UNP Q1QZR8
F	-10	ASP	-	expression tag	UNP Q1QZR8
F	-9	LEU	-	expression tag	UNP Q1QZR8
F	-8	GLY	-	expression tag	UNP Q1QZR8
F	-7	THR	-	expression tag	UNP Q1QZR8
F	-6	GLU	-	expression tag	UNP Q1QZR8
F	-5	ASN	-	expression tag	UNP Q1QZR8
F	-4	LEU	-	expression tag	UNP Q1QZR8
F	-3	TYR	-	expression tag	UNP Q1QZR8
F	-2	PHE	-	expression tag	UNP Q1QZR8
F	-1	GLN	-	expression tag	UNP Q1QZR8
F	0	SER	-	expression tag	UNP Q1QZR8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

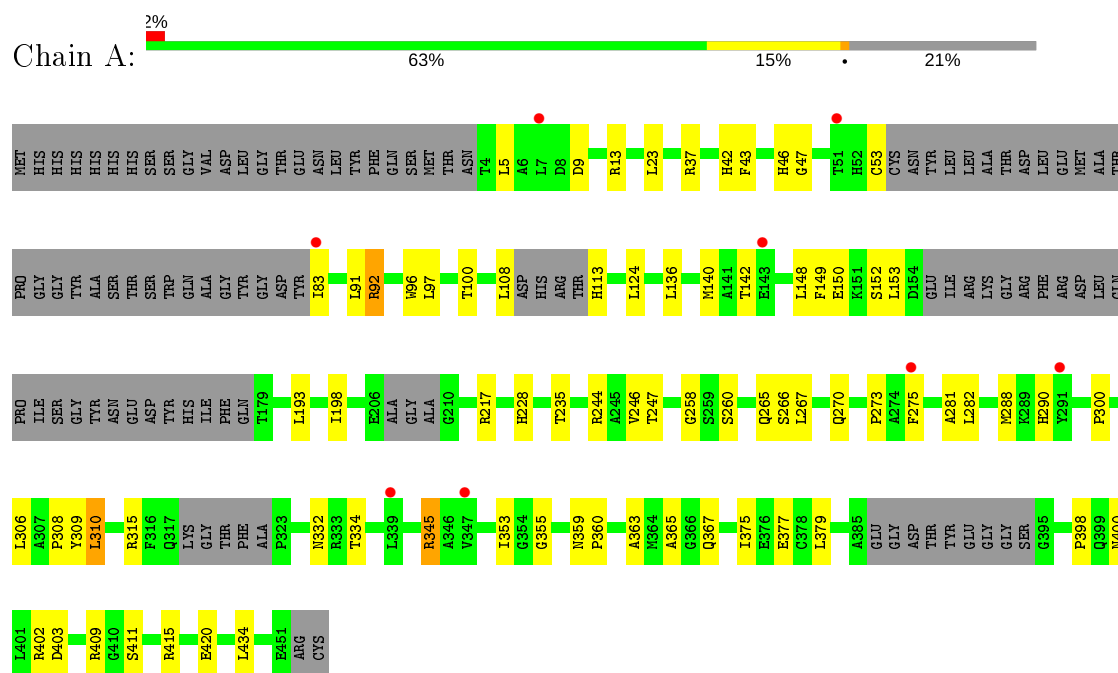
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	11	Total O 11 11	0	0
3	C	11	Total O 11 11	0	0
3	D	13	Total O 13 13	0	0
3	E	7	Total O 8 8	0	1
3	F	8	Total O 8 8	0	0

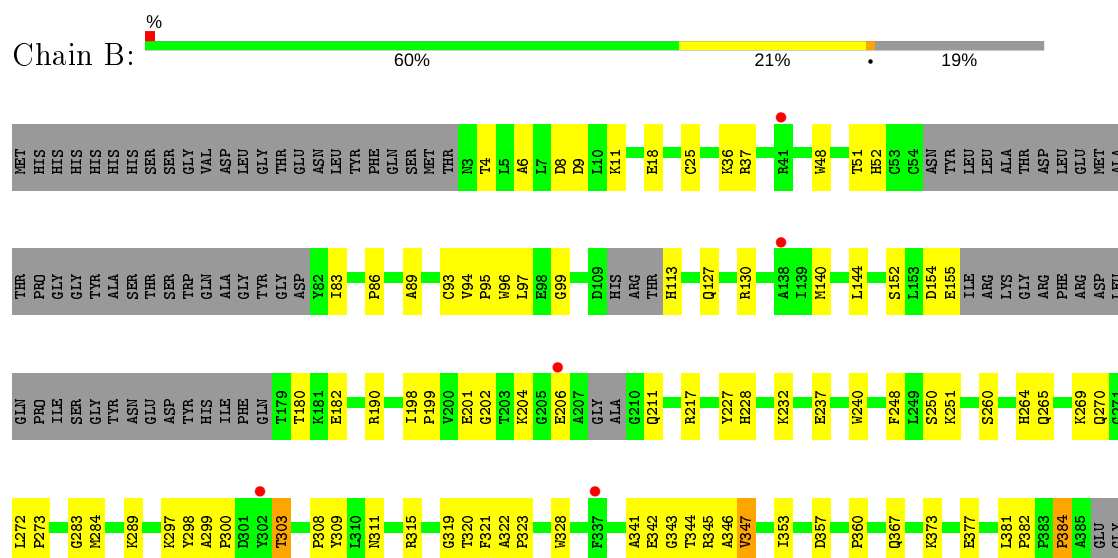
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

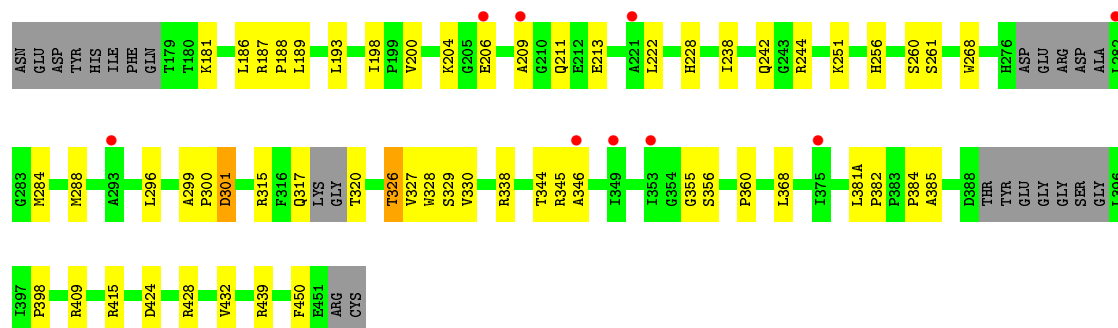
- Molecule 1: L-glutamine synthetase



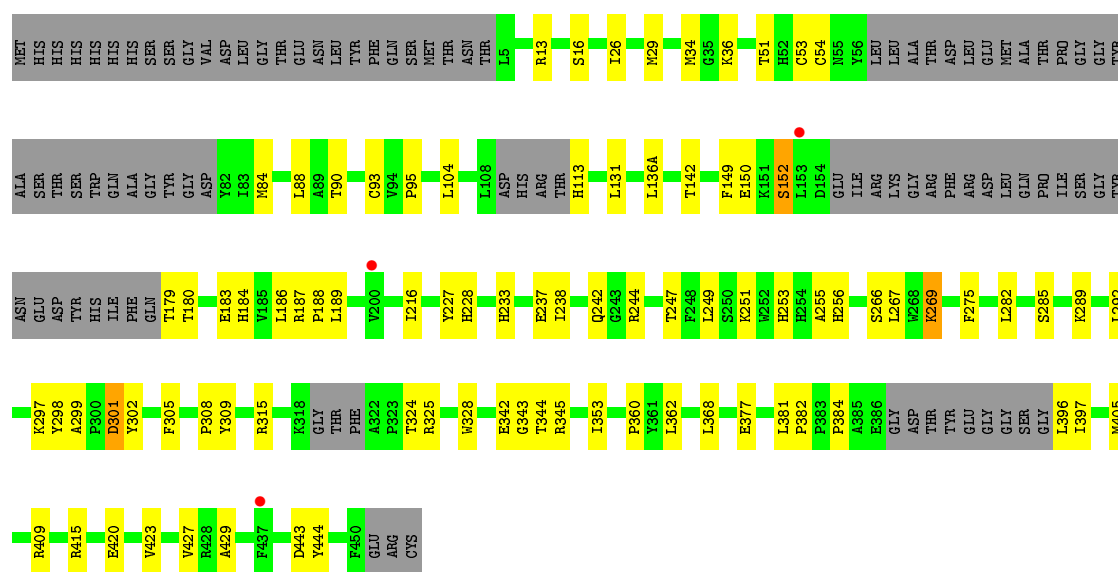
- Molecule 1: L-glutamine synthetase







• Molecule 1: L-glutamine synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.98Å 221.34Å 199.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.06 – 2.60 113.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.06-2.60) 99.9 (113.99-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.201 , 0.274 0.202 , 0.272	Depositor DCC
R_{free} test set	4515 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17834	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/2918	0.59	0/3953
1	B	0.45	0/3022	0.62	0/4093
1	C	0.45	0/3080	0.61	0/4178
1	D	0.46	0/3026	0.59	0/4100
1	E	0.44	0/2984	0.60	0/4046
1	F	0.43	0/2951	0.59	0/4004
All	All	0.45	0/17981	0.60	0/24374

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 [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	2859	0	2772	48	0
1	B	2960	0	2868	60	1
1	C	3014	0	2890	45	0
1	D	2964	0	2880	49	0
1	E	2925	0	2814	51	0
1	F	2890	0	2789	59	0
2	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	0	0
2	C	27	0	12	2	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	1	0
3	A	9	0	0	1	0
3	B	11	0	0	0	0
3	C	11	0	0	0	0
3	D	13	0	0	0	0
3	E	8	0	0	0	0
3	F	8	0	0	1	0
All	All	17834	0	17085	302	1

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 9.

All (302) 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:A:142:THR:HG21	1:A:228:HIS:HD2	1.34	0.92
1:D:315:ARG:NH2	1:D:353:ILE:O	2.09	0.85
1:A:142:THR:HG21	1:A:228:HIS:CD2	2.12	0.85
1:E:415:ARG:NH2	1:E:424:ASP:OD1	2.13	0.81
1:C:51:THR:HB	1:C:84:MET:HB2	1.66	0.77
1:A:315:ARG:NH2	1:A:353:ILE:O	2.19	0.76
1:E:109:ASP:HB3	1:E:113:HIS:HA	1.69	0.75
1:E:330:VAL:O	1:E:338:ARG:NH1	2.19	0.74
1:D:142:THR:OG1	1:D:228:HIS:HD2	1.71	0.73
1:E:123:ILE:HG23	1:E:126:ARG:HH12	1.55	0.72
1:A:400:ASN:ND2	1:A:403:ASP:OD2	2.22	0.72
1:F:113:HIS:ND1	1:F:113:HIS:O	2.24	0.71
1:A:83:ILE:HG23	1:A:108:LEU:HB2	1.72	0.70
1:B:36:LYS:NZ	1:B:52:HIS:O	2.24	0.70
1:B:315:ARG:NH2	1:B:353:ILE:O	2.25	0.69
1:F:53:CYS:SG	1:F:54:CYS:N	2.65	0.69
1:A:150:GLU:H	1:A:150:GLU:CD	1.96	0.69
1:F:13:ARG:HA	1:F:16:SER:HB3	1.76	0.67
1:D:409:ARG:O	1:D:415:ARG:NH1	2.27	0.67
1:B:182:GLU:OE2	1:C:37:ARG:NH2	2.18	0.67
1:B:154:ASP:OD1	1:B:155:GLU:N	2.28	0.67
1:C:45:ASP:HB3	1:C:46[A]:HIS:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLU:OE1	1:E:37:ARG:NH1	2.27	0.66
1:F:405:MET:SD	1:F:409:ARG:NH1	2.68	0.66
1:B:373:LYS:HE3	1:B:377:GLU:OE2	1.95	0.66
1:B:269:LYS:O	1:B:272:LEU:HB2	1.96	0.66
1:D:144:LEU:HD13	1:D:228:HIS:NE2	2.11	0.65
1:D:283:GLY:HA3	1:D:343:GLY:HA2	1.79	0.65
1:F:247:THR:HG21	1:F:249:LEU:HD12	1.79	0.64
1:D:260:SER:HA	1:D:355:GLY:HA2	1.80	0.64
1:B:344:THR:O	1:B:347:VAL:HG23	1.97	0.63
1:F:228:HIS:ND1	1:F:360:PRO:HG3	2.13	0.63
1:E:139:ILE:HD12	1:E:268:TRP:CD1	2.34	0.62
1:A:260:SER:HA	1:A:355:GLY:HA2	1.81	0.62
1:E:123:ILE:HG23	1:E:126:ARG:NH1	2.15	0.62
1:F:131:LEU:HD11	1:F:368:LEU:HD22	1.80	0.62
1:B:283:GLY:HA3	1:B:343:GLY:HA2	1.82	0.62
1:B:406:GLU:HA	1:B:409:ARG:HB3	1.81	0.62
1:C:36:LYS:HD2	1:C:51:THR:HG21	1.82	0.62
1:F:251:LYS:NZ	1:F:256:HIS:O	2.31	0.62
1:D:249:LEU:HD23	1:D:252:TRP:HA	1.81	0.61
1:E:329:SER:OG	1:E:330:VAL:N	2.33	0.61
1:C:260:SER:HA	1:C:355:GLY:HA2	1.83	0.60
1:B:113:HIS:O	1:B:113:HIS:ND1	2.32	0.60
1:A:377:GLU:HB2	1:A:379:LEU:HG	1.83	0.60
1:E:260:SER:HA	1:E:355:GLY:HA2	1.84	0.59
1:B:206:GLU:HB2	1:B:211:GLN:HB3	1.83	0.59
1:D:228:HIS:ND1	1:D:360:PRO:HG3	2.17	0.58
1:D:373:LYS:HG3	1:D:413:MET:HG2	1.85	0.58
1:E:228:HIS:ND1	1:E:360:PRO:HG3	2.18	0.58
1:F:315:ARG:NH2	1:F:353:ILE:O	2.36	0.58
1:D:87:ASP:O	1:D:90:THR:OG1	2.15	0.58
1:F:149:PHE:HE2	1:F:247:THR:HG1	1.50	0.58
1:B:93:CYS:O	1:B:95:PRO:HD3	2.04	0.57
1:F:381:LEU:HD12	1:F:382:PRO:HD2	1.86	0.57
1:B:344:THR:HG22	1:B:346:ALA:H	1.70	0.56
1:D:328:TRP:CE2	1:D:384:PRO:HB3	2.41	0.56
1:A:96:TRP:O	1:A:97:LEU:HD12	2.04	0.56
1:F:247:THR:HG22	1:F:249:LEU:H	1.70	0.56
1:B:52:HIS:ND1	2:F:501:ADP:O1B	2.38	0.56
1:A:332:ASN:HD21	1:A:334:THR:HB	1.69	0.56
1:D:403:ASP:O	1:D:406:GLU:HG2	2.06	0.56
1:D:332:ASN:OD1	1:D:333:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:LEU:HD21	1:F:328:TRP:CG	2.42	0.55
1:B:8:ASP:HA	1:B:11:LYS:HB3	1.87	0.55
1:D:183:GLU:HG3	1:D:187:ARG:HB2	1.88	0.55
1:A:273:PRO:HG3	1:A:345:ARG:HD2	1.89	0.55
1:B:199:PRO:HB2	1:B:217:ARG:HB3	1.89	0.55
1:D:292:LEU:HD13	1:D:349:ILE:HG12	1.88	0.55
1:A:266:SER:HA	1:A:275:PHE:CE2	2.42	0.54
1:E:409:ARG:O	1:E:415:ARG:NH1	2.40	0.54
1:F:297:LYS:HD3	1:F:298:TYR:CZ	2.42	0.54
1:B:36:LYS:HZ3	1:B:51:THR:HG22	1.73	0.54
1:D:415:ARG:NH2	1:D:424:ASP:OD1	2.41	0.54
1:A:300:PRO:HB3	1:A:398:PRO:HD3	1.89	0.54
1:B:190:ARG:HD2	1:B:202:GLY:HA2	1.90	0.54
1:E:261:SER:HB2	1:E:356:SER:HA	1.89	0.53
1:A:308:PRO:HG2	1:A:309:TYR:CE2	2.42	0.53
1:A:402:ARG:HG3	1:A:434:LEU:HD22	1.91	0.53
1:A:113:HIS:O	1:A:113:HIS:ND1	2.42	0.53
1:C:328:TRP:CZ2	1:C:384:PRO:HG3	2.44	0.53
1:F:328:TRP:CZ2	1:F:384:PRO:HG3	2.44	0.53
1:A:306:LEU:HD13	1:A:353:ILE:HB	1.91	0.52
1:B:228:HIS:ND1	1:B:360:PRO:HG3	2.25	0.52
1:F:142:THR:OG1	1:F:228:HIS:HD2	1.91	0.52
1:A:124:LEU:HA	1:A:365:ALA:HB2	1.92	0.52
1:C:140:MET:CE	1:C:265:GLN:HB3	2.40	0.52
1:C:293:ALA:HB1	1:C:379:LEU:HG	1.92	0.52
1:E:284:MET:HG3	1:E:288:MET:SD	2.49	0.52
1:E:39:HIS:HE1	1:E:41:ARG:HG3	1.75	0.52
1:A:149:PHE:HE2	1:A:247:THR:HG22	1.75	0.52
1:A:43:PHE:HA	1:A:47:GLY:HA3	1.91	0.52
1:C:49:GLU:O	1:C:86:PRO:HD2	2.10	0.52
1:D:316:PHE:HB3	1:D:324:THR:HG21	1.91	0.52
1:E:327:VAL:HG21	1:E:385:ALA:HB3	1.92	0.52
1:E:328:TRP:CZ2	1:E:384:PRO:HG3	2.44	0.51
1:C:185:VAL:O	1:C:188:PRO:HD2	2.09	0.51
1:F:344:THR:HG22	1:F:345:ARG:H	1.76	0.51
1:A:9:ASP:O	1:A:13:ARG:HG2	2.10	0.51
1:F:415:ARG:HD3	1:F:420:GLU:OE1	2.11	0.51
1:B:198:ILE:HD12	1:B:227:TYR:CD1	2.46	0.51
1:C:326:THR:HG22	1:C:326:THR:O	2.10	0.51
1:C:94:VAL:HG11	1:C:97:LEU:HD12	1.92	0.50
1:D:259:SER:HB3	1:D:356:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TRP:O	1:B:86:PRO:HG2	2.11	0.50
1:E:317:GLN:C	1:E:320:THR:HA	2.32	0.50
1:F:184:HIS:O	1:F:242:GLN:NE2	2.44	0.50
1:C:131:LEU:HB3	1:C:372:ILE:HD11	1.93	0.50
1:C:92:ARG:NH1	1:C:196:ALA:O	2.43	0.50
1:B:37:ARG:HH12	1:F:186:LEU:HD12	1.75	0.50
1:D:418:MET:HB3	1:D:422:VAL:HG21	1.94	0.50
1:B:284:MET:HE1	1:B:328:TRP:CH2	2.46	0.49
1:D:326:THR:HG22	1:D:396:LEU:N	2.27	0.49
1:F:305:PHE:CD1	1:F:362:LEU:HB3	2.47	0.49
1:E:142:THR:OG1	1:E:228:HIS:HD2	1.95	0.49
1:F:188:PRO:HG2	1:F:242:GLN:HE21	1.77	0.49
1:D:93:CYS:O	1:D:95:PRO:HD3	2.13	0.49
1:C:140:MET:HE2	1:C:265:GLN:HB3	1.95	0.49
1:E:204:LYS:HE2	1:F:36:LYS:HE2	1.95	0.49
1:A:363:ALA:O	1:A:367:GLN:HG3	2.12	0.49
1:B:6:ALA:HB3	1:B:9:ASP:HB2	1.95	0.49
1:B:18:GLU:O	1:B:99:GLY:HA2	2.12	0.49
1:C:140:MET:SD	1:C:364:MET:HE2	2.53	0.49
1:C:147:PHE:CE2	1:C:252:TRP:HD1	2.31	0.49
1:B:144:LEU:HD21	1:B:232:LYS:HG3	1.96	0.48
1:B:201:GLU:HG2	1:C:42:HIS:CD2	2.49	0.48
1:B:328:TRP:CH2	1:B:384:PRO:HG3	2.48	0.48
1:B:36:LYS:NZ	1:B:51:THR:HG22	2.29	0.48
1:F:325:ARG:HA	1:F:396:LEU:HD12	1.94	0.48
1:B:289:LYS:CB	1:B:381:LEU:HD11	2.44	0.48
1:A:148:LEU:HD22	1:A:244:ARG:HD2	1.95	0.48
1:A:228:HIS:ND1	1:A:360:PRO:HG3	2.29	0.48
1:E:152:SER:OG	1:E:153:LEU:N	2.47	0.48
1:E:143:GLU:HB3	1:E:213:GLU:OE2	2.13	0.48
1:C:253:HIS:HB3	1:C:256:HIS:ND1	2.29	0.47
1:C:322:ALA:O	1:C:324:THR:N	2.48	0.47
1:A:152:SER:OG	1:A:153:LEU:N	2.48	0.47
1:B:328:TRP:CZ2	1:B:384:PRO:HG3	2.50	0.47
1:A:140:MET:CE	1:A:265:GLN:HB3	2.44	0.47
1:A:415:ARG:HD3	1:A:420:GLU:OE1	2.14	0.47
1:C:295:LEU:O	1:C:299:ALA:HB2	2.14	0.47
1:D:299:ALA:HA	1:D:302:TYR:CE2	2.49	0.47
1:D:423:VAL:O	1:D:427:VAL:HG23	2.15	0.47
1:A:411:SER:O	1:A:415:ARG:HG3	2.14	0.47
1:C:364:MET:O	1:C:368:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:HIS:HB3	1:A:375:ILE:HA	1.97	0.47
1:F:183:GLU:HG3	1:F:187:ARG:HB2	1.97	0.47
1:D:301:ASP:OD1	1:D:301:ASP:N	2.48	0.47
1:D:8:ASP:N	1:D:8:ASP:OD1	2.47	0.47
1:B:204:LYS:HE2	1:B:204:LYS:HB3	1.64	0.46
1:B:127:GLN:HA	1:B:130:ARG:HG3	1.96	0.46
1:F:324:THR:HG23	1:F:397:ILE:HG12	1.98	0.46
1:F:443:ASP:OD1	1:F:444:TYR:N	2.48	0.46
1:C:26:ILE:HD11	1:C:56:TYR:CD2	2.51	0.46
1:F:299:ALA:HA	1:F:302:TYR:CZ	2.50	0.46
1:F:93:CYS:O	1:F:95:PRO:HD3	2.15	0.46
1:A:359:ASN:HA	1:A:360:PRO:HD3	1.83	0.46
1:D:381:LEU:HD12	1:D:382:PRO:HD2	1.98	0.46
1:B:180:THR:HG21	1:C:241:GLN:HE21	1.80	0.46
1:B:250:SER:OG	1:B:357:ASP:OD2	2.27	0.46
1:B:4:THR:HG21	1:B:89:ALA:O	2.14	0.46
1:D:328:TRP:CZ2	1:D:384:PRO:HB3	2.50	0.46
1:B:52:HIS:CD2	1:B:83:ILE:HG13	2.51	0.46
1:E:344:THR:C	1:E:346:ALA:H	2.19	0.46
1:A:332:ASN:ND2	1:A:334:THR:HB	2.30	0.46
1:E:193:LEU:HD22	1:E:198:ILE:HG13	1.98	0.46
1:C:329:SER:O	1:C:338:ARG:HA	2.16	0.45
1:F:285:SER:O	1:F:289:LYS:HG3	2.16	0.45
1:A:275:PHE:HA	1:A:288:MET:HB2	1.97	0.45
1:E:198:ILE:O	1:E:200:VAL:HG23	2.16	0.45
1:E:381(A):LEU:HA	1:E:382:PRO:HD3	1.82	0.45
1:D:372:ILE:O	1:D:376:GLU:HG3	2.16	0.45
1:C:344:THR:C	1:C:346:ALA:H	2.20	0.45
1:B:94:VAL:HG13	1:B:96:TRP:CE2	2.51	0.45
1:D:397:ILE:HG12	1:D:398:PRO:HD2	1.98	0.45
1:F:150:GLU:O	1:F:244:ARG:NH1	2.48	0.45
1:F:29:MET:HE1	1:F:429:ALA:HB1	1.98	0.45
1:D:121:ARG:NH1	1:D:226:ASP:OD1	2.50	0.45
1:F:328:TRP:CH2	1:F:384:PRO:HG3	2.51	0.45
1:E:301:ASP:OD1	1:E:301:ASP:N	2.50	0.45
1:E:11:LYS:HE2	1:E:44:VAL:HB	1.98	0.45
1:B:94:VAL:HG13	1:B:96:TRP:CZ2	2.52	0.45
1:D:92:ARG:NH1	1:D:196:ALA:O	2.41	0.45
1:E:238:ILE:O	1:E:242:GLN:HG2	2.17	0.45
1:B:273:PRO:HG3	1:B:345:ARG:HG3	1.99	0.45
1:F:377:GLU:OE2	3:F:601:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ALA:O	1:B:9:ASP:HB3	2.17	0.44
1:C:423:VAL:O	1:C:427:VAL:HG13	2.16	0.44
1:D:144:LEU:HD13	1:D:228:HIS:HE2	1.83	0.44
1:B:37:ARG:NH1	1:F:186:LEU:HD12	2.32	0.44
1:B:94:VAL:HG11	1:B:97:LEU:HD12	1.98	0.44
1:E:296:LEU:HD11	1:E:328:TRP:CD1	2.53	0.44
1:B:299:ALA:HB3	1:B:300:PRO:HD3	1.99	0.44
1:D:418:MET:HB3	1:D:422:VAL:CG2	2.48	0.44
1:F:216:ILE:HD13	1:F:227:TYR:HB3	2.00	0.44
1:A:92:ARG:NH2	3:A:601:HOH:O	2.48	0.44
1:C:283:GLY:O	1:C:347:VAL:HG21	2.18	0.44
1:A:23:LEU:CD2	1:A:37:ARG:HG2	2.48	0.44
1:A:409:ARG:HH21	1:A:409:ARG:HG3	1.83	0.44
1:E:25:CYS:HA	1:E:34:MET:O	2.17	0.44
1:A:42:HIS:CD2	1:C:201:GLU:HG2	2.53	0.44
1:B:450:PHE:HA	1:B:451:GLU:C	2.38	0.44
1:C:308:PRO:HG2	1:C:309:TYR:CE2	2.52	0.44
1:E:148:LEU:HA	1:E:148:LEU:HD12	1.85	0.44
1:F:53:CYS:HB2	1:F:84:MET:HG3	1.99	0.44
1:C:291:TYR:CE2	1:C:371:GLY:HA3	2.53	0.44
1:A:97:LEU:HD23	1:A:100:THR:HG21	2.00	0.44
1:D:94:VAL:HG22	1:D:102:MET:HG2	2.00	0.44
1:F:189:LEU:HA	1:F:238:ILE:HD13	2.00	0.44
1:A:258:GLY:HA3	1:A:315:ARG:HG3	2.00	0.44
1:A:5:LEU:HD23	1:A:91:LEU:HG	2.00	0.44
1:B:140:MET:HA	1:B:264:HIS:O	2.18	0.44
1:B:308:PRO:HG2	1:B:309:TYR:CE2	2.52	0.44
1:D:131:LEU:HG	1:D:372:ILE:HD11	1.99	0.44
1:D:39:HIS:HE1	1:D:41:ARG:HG3	1.83	0.44
1:F:342:GLU:HA	1:F:343:GLY:HA2	1.70	0.44
1:F:90:THR:HG21	1:F:104:LEU:HB2	1.99	0.43
1:E:82:TYR:HB3	1:E:107:LEU:HD11	2.00	0.43
1:C:348:ARG:HD2	2:C:501:ADP:C2	2.53	0.43
1:E:206:GLU:HG3	1:E:211:GLN:HG2	2.00	0.43
1:E:39:HIS:CE1	1:E:41:ARG:HG3	2.52	0.43
1:B:297:LYS:HE3	1:B:298:TYR:OH	2.18	0.43
1:B:341:ALA:O	1:B:344:THR:HB	2.18	0.43
1:E:222:LEU:HD12	1:E:222:LEU:HA	1.85	0.43
1:A:308:PRO:HG2	1:A:309:TYR:CD2	2.53	0.43
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.79	0.43
1:C:156:ILE:C	1:C:158:LYS:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ARG:HD2	1:C:202:GLY:HA2	2.01	0.43
1:C:260:SER:HB3	1:C:315:ARG:NH1	2.34	0.43
1:E:439:ARG:HG2	1:E:439:ARG:O	2.19	0.43
1:E:131:LEU:CD1	1:E:138:ALA:HB2	2.48	0.43
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.87	0.43
1:F:26:ILE:HG23	1:F:84:MET:HE2	1.99	0.43
1:F:36:LYS:HD2	1:F:51:THR:HG21	2.01	0.43
1:C:198:ILE:HG13	1:C:227:TYR:CD1	2.54	0.43
1:F:238:ILE:O	1:F:242:GLN:HG2	2.18	0.43
1:B:381:LEU:HA	1:B:382:PRO:HD2	1.88	0.43
1:D:130:ARG:HH12	1:D:417:ALA:CB	2.32	0.43
1:D:142:THR:OG1	1:D:228:HIS:CD2	2.61	0.43
1:E:300:PRO:HB3	1:E:398:PRO:HD3	2.01	0.43
1:F:266:SER:HA	1:F:275:PHE:CE2	2.54	0.43
1:D:285:SER:O	1:D:289:LYS:HG3	2.19	0.42
1:A:217:ARG:HB3	1:A:217:ARG:HE	1.58	0.42
1:C:149:PHE:HE2	1:C:247:THR:HG22	1.84	0.42
1:C:187:ARG:HB3	1:C:188:PRO:HD3	2.01	0.42
1:E:189:LEU:HA	1:E:238:ILE:HD12	2.00	0.42
1:F:299:ALA:HA	1:F:302:TYR:CE2	2.55	0.42
1:C:424:ASP:O	1:C:427:VAL:HG22	2.20	0.42
1:D:299:ALA:HA	1:D:302:TYR:CZ	2.55	0.42
1:F:152:SER:OG	1:F:152:SER:O	2.37	0.42
1:B:240:TRP:CZ3	1:F:180:THR:HB	2.54	0.42
1:D:96:TRP:CZ2	1:D:234:ALA:HB2	2.54	0.42
1:A:235:THR:HG22	1:A:246:VAL:HG11	2.02	0.42
1:B:265:GLN:NE2	1:B:367:GLN:OE1	2.53	0.42
1:D:147:PHE:CE1	1:D:211:GLN:HB2	2.55	0.42
1:F:308:PRO:HG2	1:F:309:TYR:CE2	2.54	0.42
1:B:251:LYS:O	1:B:311:ASN:ND2	2.44	0.42
1:D:131:LEU:HA	1:D:131:LEU:HD23	1.83	0.42
1:D:353:ILE:HD13	1:D:397:ILE:CD1	2.50	0.42
1:F:233:HIS:O	1:F:237:GLU:HG2	2.20	0.42
1:F:136(A):LEU:HD13	1:F:267:LEU:HD13	2.02	0.42
1:F:301:ASP:OD1	1:F:301:ASP:N	2.52	0.42
1:B:342:GLU:N	1:B:342:GLU:OE2	2.40	0.42
1:F:188:PRO:HG2	1:F:242:GLN:NE2	2.35	0.42
1:C:409:ARG:NH2	1:C:431:GLU:OE2	2.53	0.41
1:D:260:SER:HB3	1:D:315:ARG:NH1	2.35	0.41
1:E:187:ARG:HB3	1:E:188:PRO:HD3	2.02	0.41
1:E:368:LEU:HA	1:E:368:LEU:HD23	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ARG:HH21	2:C:501:ADP:H5'1	1.86	0.41
1:C:94:VAL:HG13	1:C:96:TRP:CZ2	2.55	0.41
1:B:232:LYS:HE3	1:B:248:PHE:CG	2.55	0.41
1:B:320:THR:O	1:B:322:ALA:N	2.50	0.41
1:E:299:ALA:HB3	1:E:300:PRO:HD3	2.02	0.41
1:A:281:ALA:C	1:A:282:LEU:HD23	2.41	0.41
1:D:146:PHE:HD2	1:D:246:VAL:HG23	1.84	0.41
1:E:296:LEU:HD11	1:E:328:TRP:HD1	1.85	0.41
1:F:53:CYS:HG	1:F:54:CYS:H	1.66	0.41
1:A:193:LEU:HD22	1:A:198:ILE:HD12	2.03	0.41
1:E:244:ARG:HD3	1:E:244:ARG:HA	1.93	0.41
1:C:118:HIS:CD2	1:C:118:HIS:H	2.37	0.41
1:E:11:LYS:HB2	1:E:11:LYS:HE3	1.69	0.41
1:E:260:SER:HB3	1:E:315:ARG:NH1	2.36	0.41
1:A:149:PHE:HE2	1:A:247:THR:CG2	2.34	0.41
1:D:379:LEU:HA	1:D:379:LEU:HD23	1.83	0.41
1:F:149:PHE:HE2	1:F:247:THR:OG1	2.04	0.41
1:B:237:GLU:OE1	1:F:179:THR:HB	2.20	0.41
1:F:253:HIS:CE1	1:F:255:ALA:H	2.39	0.41
1:A:149:PHE:O	1:A:244:ARG:HD3	2.20	0.41
1:B:405:MET:SD	1:B:431:GLU:HG3	2.61	0.41
1:D:128:LEU:O	1:D:132:GLU:HG3	2.21	0.41
1:E:428:ARG:O	1:E:432:VAL:HG12	2.21	0.41
1:F:269:LYS:HB2	1:F:269:LYS:HE2	1.84	0.41
1:E:126:ARG:O	1:E:130:ARG:HG3	2.20	0.40
1:C:10:LEU:O	1:C:14:VAL:HG23	2.21	0.40
1:E:251:LYS:HE3	1:E:256:HIS:O	2.22	0.40
1:B:423:VAL:O	1:B:427:VAL:HG23	2.21	0.40
1:E:29:MET:HG3	1:E:57:LEU:CD2	2.51	0.40
1:F:423:VAL:O	1:F:427:VAL:HG23	2.21	0.40
1:A:136:LEU:HD13	1:A:267:LEU:HD13	2.04	0.40
1:B:303:THR:HG21	1:B:398:PRO:HD2	2.03	0.40
1:E:186:LEU:HD23	1:E:186:LEU:HA	1.79	0.40
1:F:88:LEU:HD22	1:F:88:LEU:H	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ASP:OD2	1:B:444:TYR:OH[3_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/475 (76%)	348 (97%)	10 (3%)	2 (1%)	25	47
1	B	373/475 (78%)	352 (94%)	16 (4%)	5 (1%)	12	24
1	C	387/475 (82%)	360 (93%)	22 (6%)	5 (1%)	12	24
1	D	376/475 (79%)	358 (95%)	15 (4%)	3 (1%)	19	39
1	E	367/475 (77%)	339 (92%)	22 (6%)	6 (2%)	9	19
1	F	369/475 (78%)	351 (95%)	18 (5%)	0	100	100
All	All	2232/2850 (78%)	2108 (94%)	103 (5%)	21 (1%)	17	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	49	GLU
1	A	270	GLN
1	B	319	GLY
1	B	321	PHE
1	B	384	PRO
1	E	181	LYS
1	E	209	ALA
1	B	323	PRO
1	C	210	GLY
1	C	157	ARG
1	C	384	PRO
1	D	153	LEU
1	D	221	ALA
1	E	450	PHE
1	C	181	LYS
1	D	356	SER
1	A	46	HIS
1	B	347	VAL
1	E	46	HIS
1	E	326	THR

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Mol	Chain	Res	Type
1	E	345	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/386 (74%)	281 (99%)	4 (1%)	67	85
1	B	298/386 (77%)	292 (98%)	6 (2%)	55	78
1	C	297/386 (77%)	295 (99%)	2 (1%)	84	94
1	D	296/386 (77%)	291 (98%)	5 (2%)	60	81
1	E	291/386 (75%)	287 (99%)	4 (1%)	67	85
1	F	285/386 (74%)	280 (98%)	5 (2%)	59	80
All	All	1752/2316 (76%)	1726 (98%)	26 (2%)	65	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	92	ARG
1	A	310	LEU
1	A	345	ARG
1	B	25	CYS
1	B	152	SER
1	B	260	SER
1	B	270	GLN
1	B	303	THR
1	B	442	SER
1	C	9	ASP
1	C	421	ASP
1	D	53	CYS
1	D	182	GLU
1	D	285	SER
1	D	301	ASP
1	D	378	CYS

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Mol	Chain	Res	Type
1	E	25	CYS
1	E	51	THR
1	E	301	ASP
1	E	326	THR
1	F	34	MET
1	F	152	SER
1	F	269	LYS
1	F	282	LEU
1	F	301	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	B	3	ASN
1	D	228	HIS
1	E	228	HIS
1	F	184	HIS
1	F	228	HIS
1	F	242	GLN
1	F	265	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	C	501	-	24,29,29	1.00	1 (4%)	29,45,45	1.35	3 (10%)
2	ADP	A	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.47	4 (13%)
2	ADP	F	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	3 (10%)
2	ADP	D	501	-	24,29,29	0.89	1 (4%)	29,45,45	1.29	3 (10%)
2	ADP	B	501	-	24,29,29	1.00	2 (8%)	29,45,45	1.44	3 (10%)
2	ADP	E	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.24	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	501	-	-	2/12/32/32	0/3/3/3
2	ADP	A	501	-	-	7/12/32/32	0/3/3/3
2	ADP	F	501	-	-	3/12/32/32	0/3/3/3
2	ADP	D	501	-	-	7/12/32/32	0/3/3/3
2	ADP	B	501	-	-	3/12/32/32	0/3/3/3
2	ADP	E	501	-	-	3/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	ADP	C5-C4	2.64	1.47	1.40
2	A	501	ADP	C5-C4	2.54	1.47	1.40
2	F	501	ADP	C5-C4	2.42	1.47	1.40
2	B	501	ADP	C5-C4	2.40	1.47	1.40
2	E	501	ADP	C5-C4	2.39	1.47	1.40
2	D	501	ADP	C5-C4	2.31	1.47	1.40
2	B	501	ADP	C2-N3	2.00	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ADP	N3-C2-N1	-3.91	122.57	128.68
2	F	501	ADP	PA-O3A-PB	-3.79	119.83	132.83
2	B	501	ADP	PA-O3A-PB	-3.69	120.16	132.83
2	B	501	ADP	N3-C2-N1	-3.58	123.08	128.68
2	A	501	ADP	PA-O3A-PB	-3.49	120.84	132.83
2	C	501	ADP	N3-C2-N1	-3.44	123.31	128.68
2	F	501	ADP	N3-C2-N1	-3.36	123.42	128.68
2	D	501	ADP	N3-C2-N1	-3.18	123.70	128.68
2	E	501	ADP	N3-C2-N1	-3.17	123.73	128.68
2	F	501	ADP	C4-C5-N7	-3.06	106.21	109.40
2	D	501	ADP	C4-C5-N7	-3.00	106.28	109.40
2	C	501	ADP	PA-O3A-PB	-2.93	122.76	132.83
2	B	501	ADP	C4-C5-N7	-2.84	106.44	109.40
2	A	501	ADP	C4-C5-N7	-2.82	106.45	109.40
2	E	501	ADP	C4-C5-N7	-2.76	106.52	109.40
2	C	501	ADP	C4-C5-N7	-2.36	106.94	109.40
2	E	501	ADP	PA-O3A-PB	-2.30	124.93	132.83
2	D	501	ADP	PA-O3A-PB	-2.26	125.09	132.83
2	A	501	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	ADP	O4'-C4'-C5'-O5'
2	A	501	ADP	PA-O3A-PB-O3B
2	A	501	ADP	PB-O3A-PA-O5'
2	A	501	ADP	C5'-O5'-PA-O1A
2	A	501	ADP	C5'-O5'-PA-O2A
2	F	501	ADP	PB-O3A-PA-O5'
2	F	501	ADP	C5'-O5'-PA-O1A
2	D	501	ADP	C5'-O5'-PA-O2A
2	D	501	ADP	O4'-C4'-C5'-O5'
2	D	501	ADP	C3'-C4'-C5'-O5'
2	E	501	ADP	C5'-O5'-PA-O1A
2	E	501	ADP	C5'-O5'-PA-O2A
2	E	501	ADP	C5'-O5'-PA-O3A
2	C	501	ADP	C3'-C4'-C5'-O5'
2	D	501	ADP	PB-O3A-PA-O5'
2	F	501	ADP	PA-O3A-PB-O1B
2	A	501	ADP	C5'-O5'-PA-O3A
2	D	501	ADP	C5'-O5'-PA-O3A
2	D	501	ADP	C5'-O5'-PA-O1A

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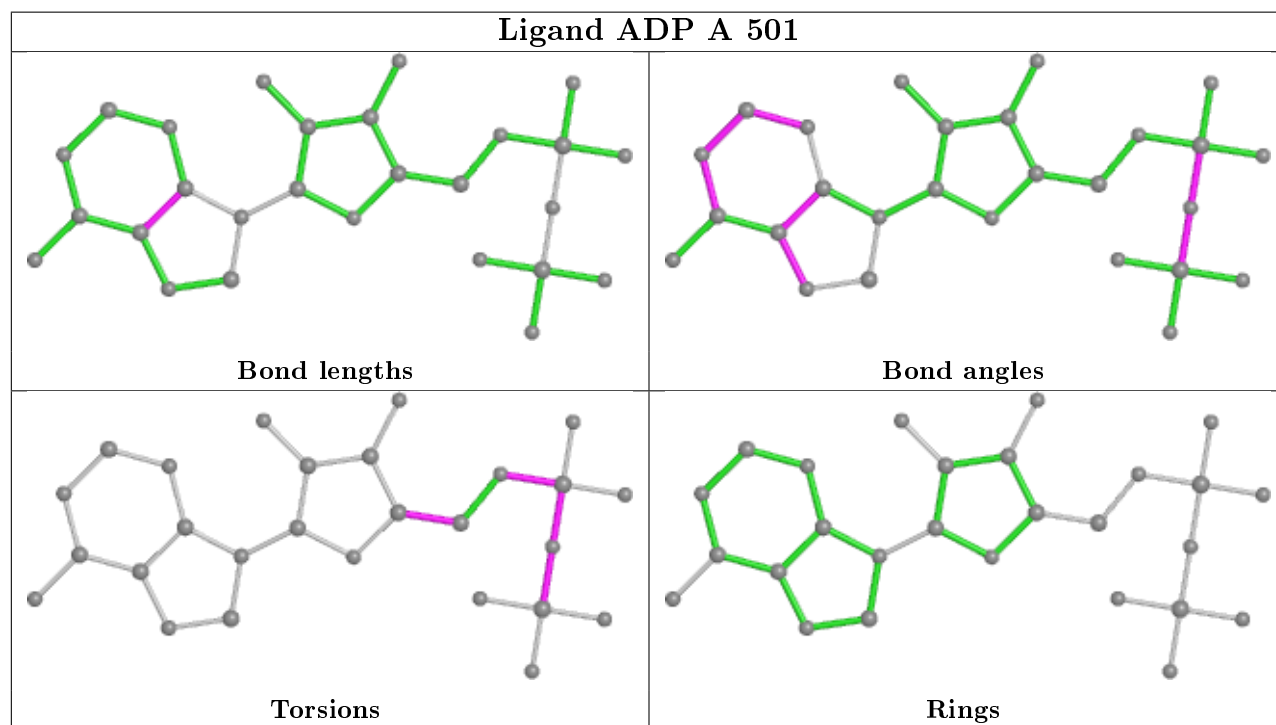
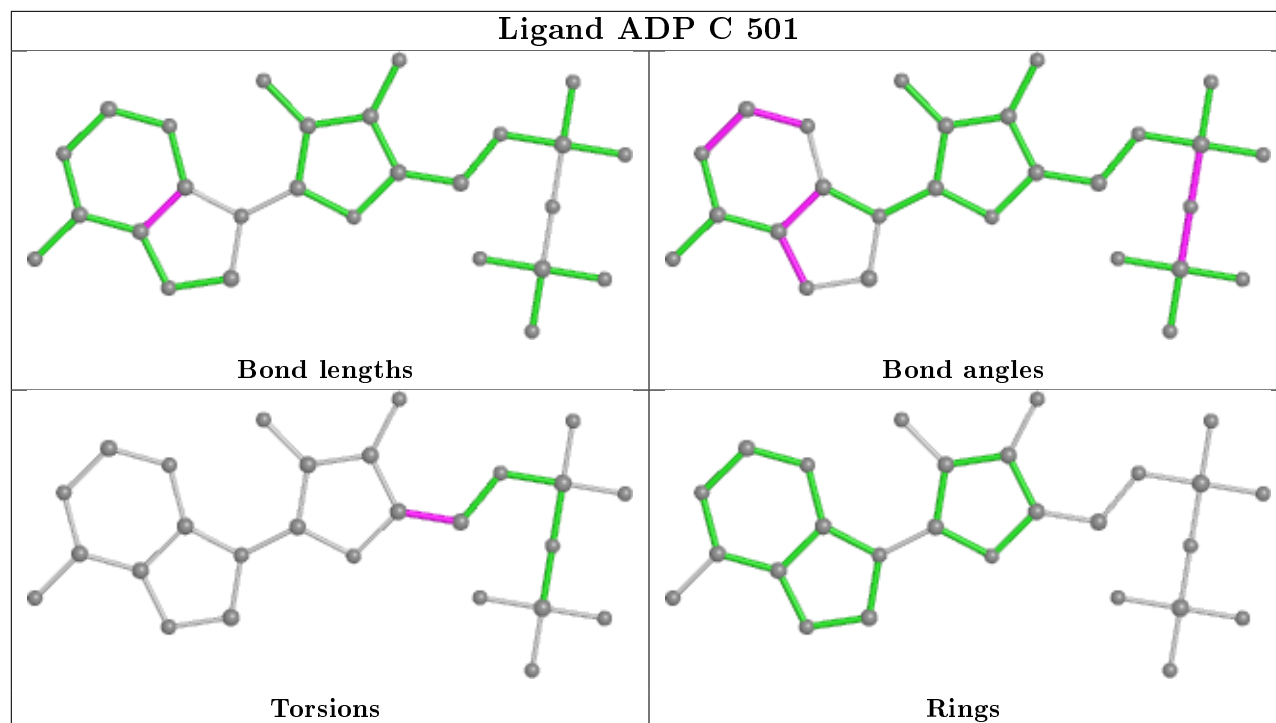
Mol	Chain	Res	Type	Atoms
2	B	501	ADP	PB-O3A-PA-O1A
2	A	501	ADP	O4'-C4'-C5'-O5'
2	A	501	ADP	C3'-C4'-C5'-O5'
2	B	501	ADP	C5'-O5'-PA-O3A
2	D	501	ADP	PB-O3A-PA-O1A
2	B	501	ADP	PB-O3A-PA-O2A

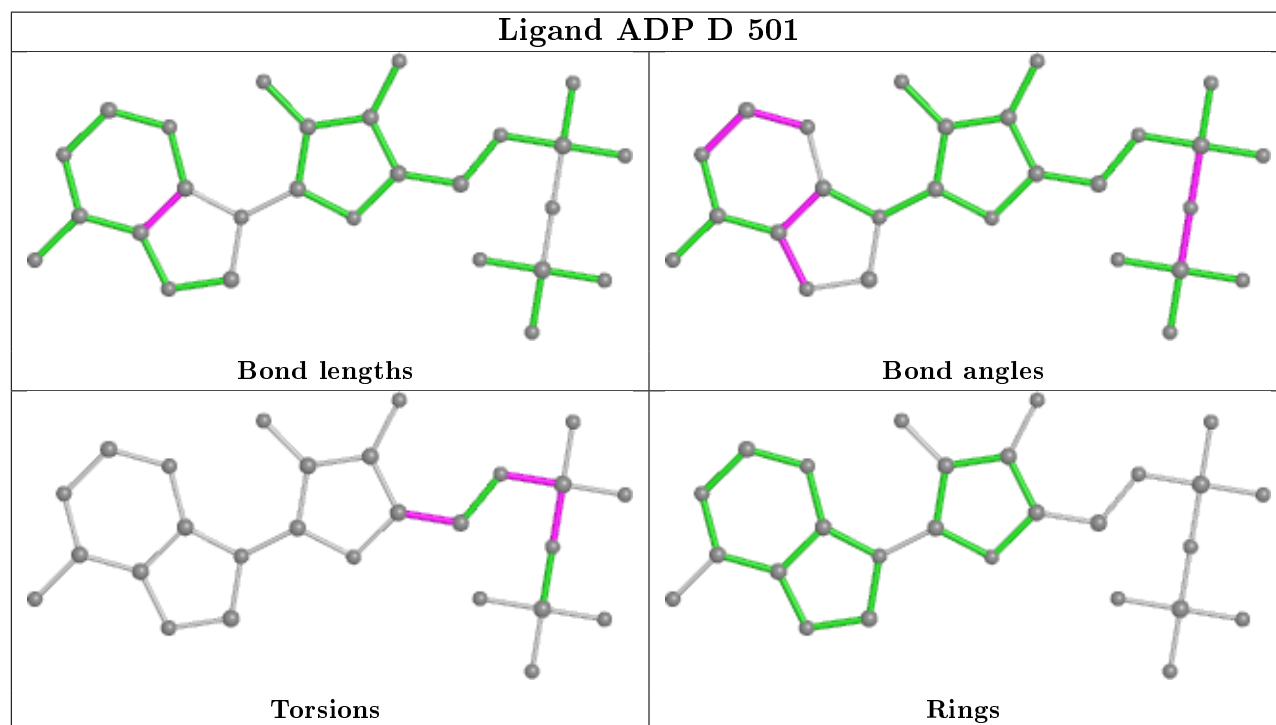
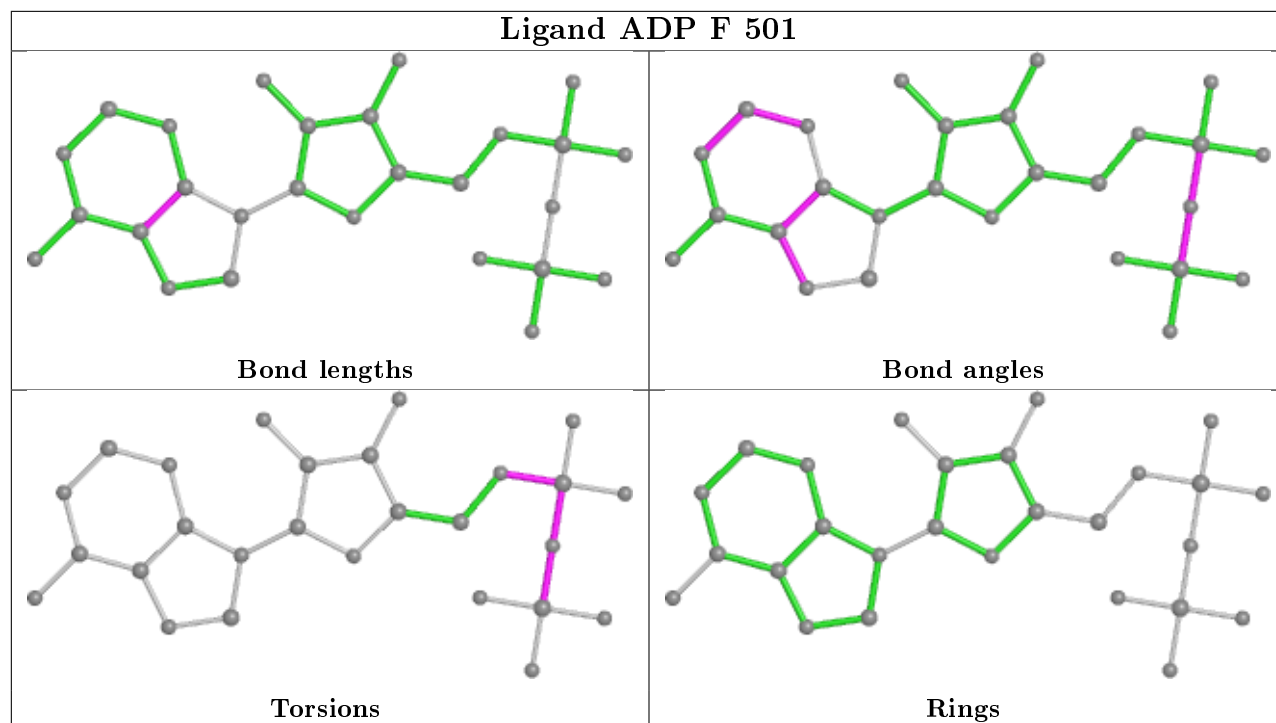
There are no ring outliers.

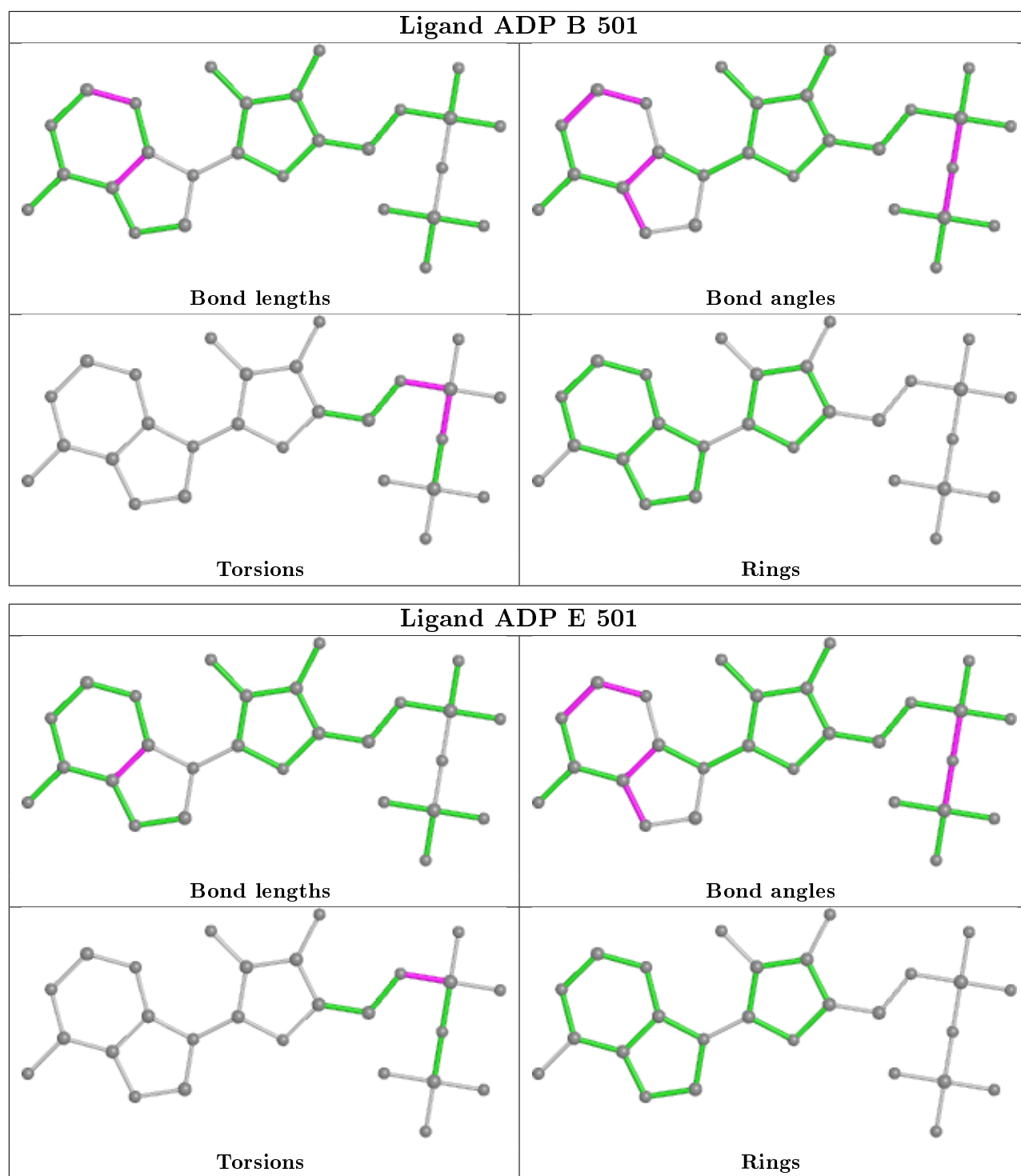
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	ADP	2	0
2	F	501	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 than 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.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	374/475 (78%)	0.08	8 (2%) 63 58	35, 58, 91, 127	0
1	B	385/475 (81%)	0.08	5 (1%) 77 73	36, 58, 92, 119	0
1	C	396/475 (83%)	0.04	7 (1%) 68 64	33, 55, 95, 133	0
1	D	386/475 (81%)	0.04	7 (1%) 68 64	32, 53, 87, 126	0
1	E	383/475 (80%)	0.05	11 (2%) 51 45	36, 60, 96, 148	0
1	F	381/475 (80%)	0.02	3 (0%) 86 84	37, 57, 90, 116	0
All	All	2305/2850 (80%)	0.05	41 (1%) 68 64	32, 56, 93, 148	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	386	GLU	7.6
1	A	51	THR	3.2
1	C	349	ILE	3.1
1	A	291	TYR	2.9
1	D	349	ILE	2.8
1	E	56	TYR	2.8
1	E	206	GLU	2.7
1	B	206	GLU	2.7
1	C	275	PHE	2.6
1	E	293	ALA	2.6
1	D	339	LEU	2.5
1	C	292	LEU	2.5
1	F	153	LEU	2.5
1	A	347	VAL	2.4
1	A	143	GLU	2.4
1	D	330	VAL	2.4
1	D	247	THR	2.4
1	E	375	ILE	2.3
1	C	339	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	302	TYR	2.3
1	E	209	ALA	2.3
1	D	56	TYR	2.3
1	F	437	PHE	2.3
1	A	339	LEU	2.2
1	B	337	PHE	2.2
1	B	138	ALA	2.2
1	A	7	LEU	2.2
1	C	288	MET	2.2
1	E	58	LEU	2.2
1	E	282	LEU	2.2
1	C	289	LYS	2.2
1	E	349	ILE	2.2
1	E	221	ALA	2.1
1	D	316	PHE	2.1
1	F	200	VAL	2.1
1	A	83	ILE	2.1
1	E	346	ALA	2.1
1	A	275	PHE	2.0
1	B	41	ARG	2.0
1	C	347	VAL	2.0
1	E	353	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

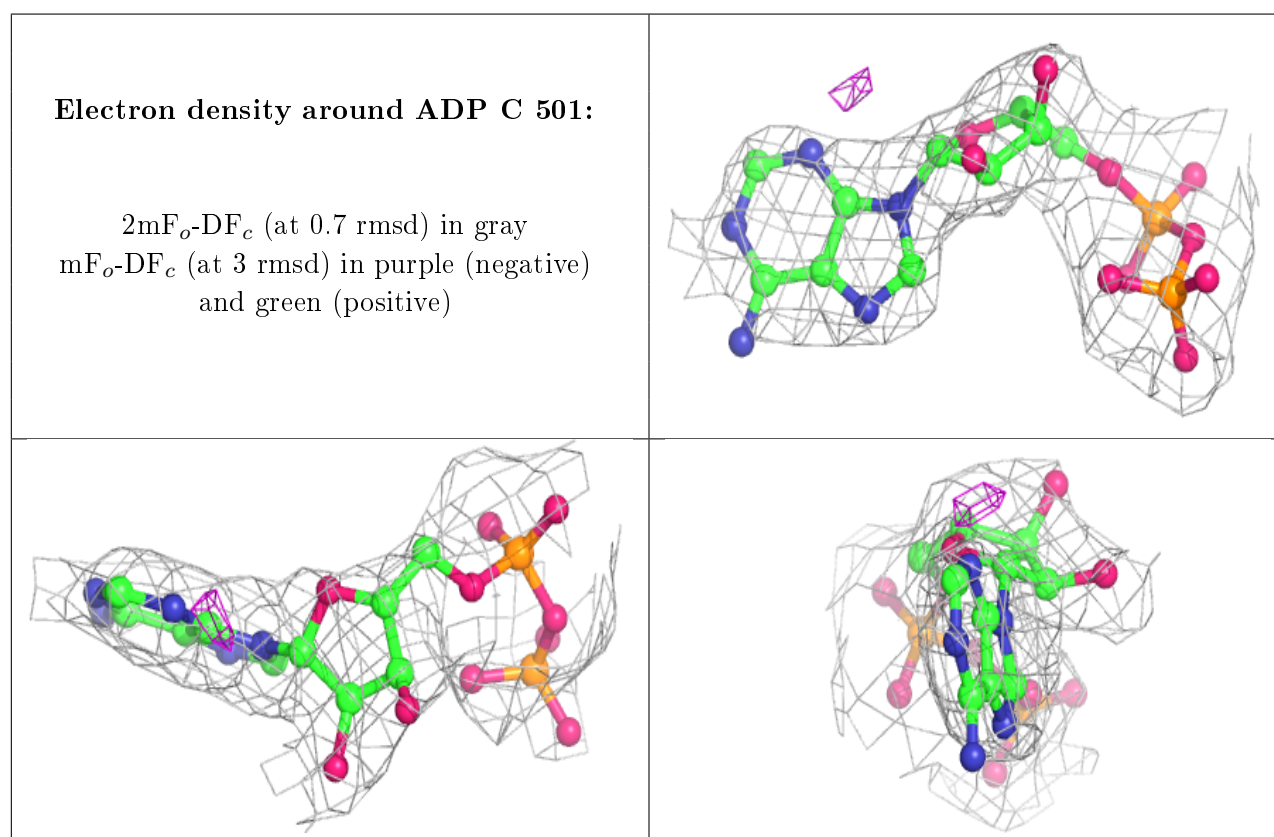
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	C	501	27/27	0.84	0.21	71,85,167,189	0

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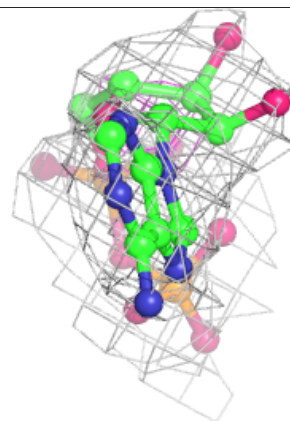
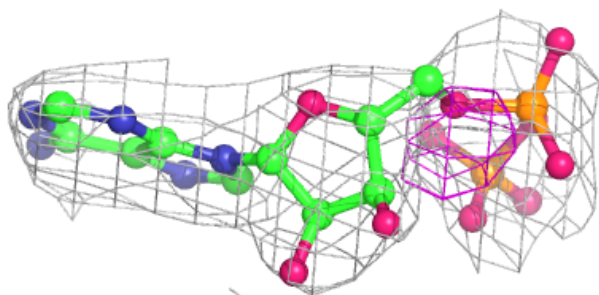
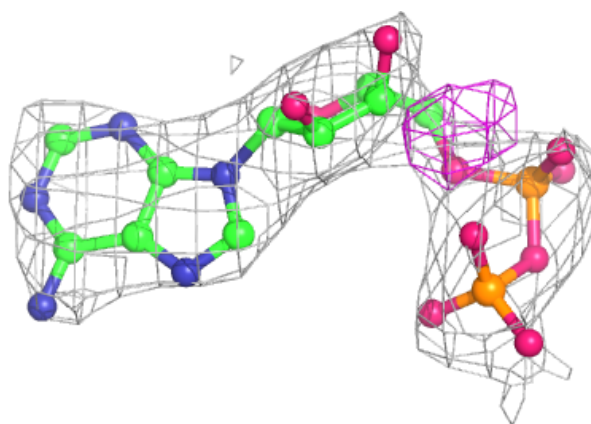
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	F	501	27/27	0.87	0.25	69,81,154,172	0
2	ADP	A	501	27/27	0.88	0.21	64,77,148,194	0
2	ADP	D	501	27/27	0.89	0.22	54,76,182,184	0
2	ADP	E	501	27/27	0.91	0.23	66,77,127,141	0
2	ADP	B	501	27/27	0.92	0.19	45,61,141,142	0

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.

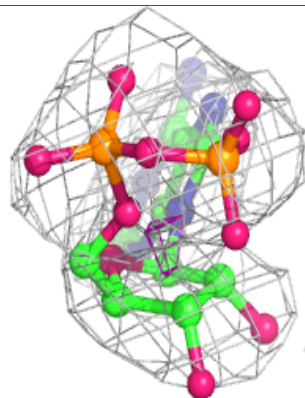
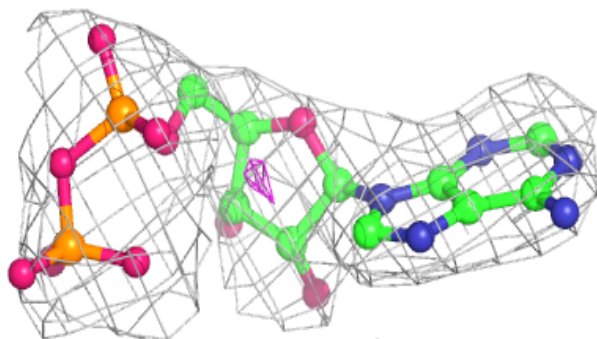
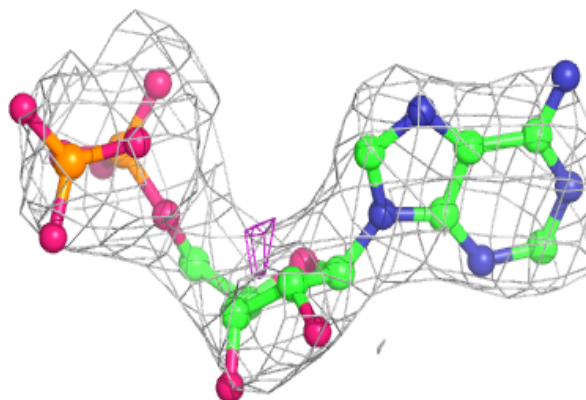


Electron density around ADP F 501:

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

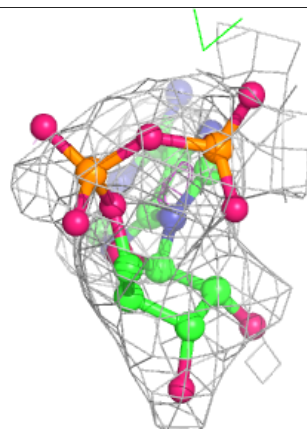
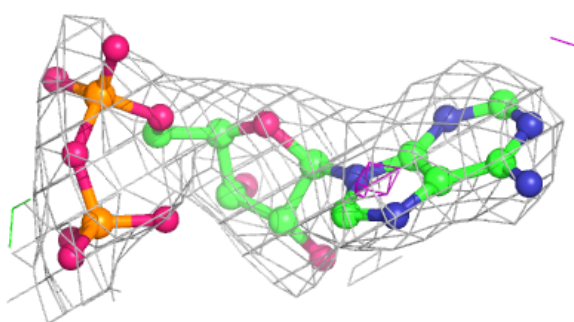
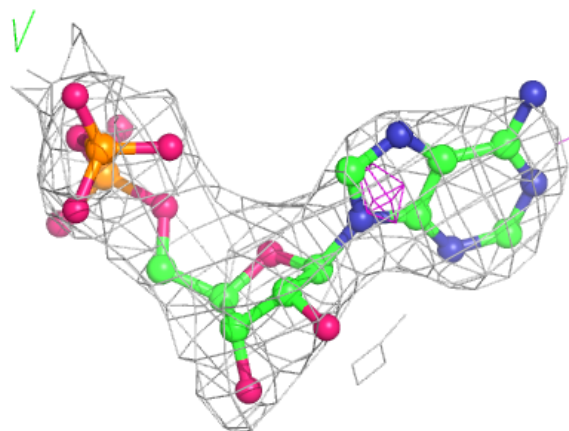
**Electron density around ADP A 501:**

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

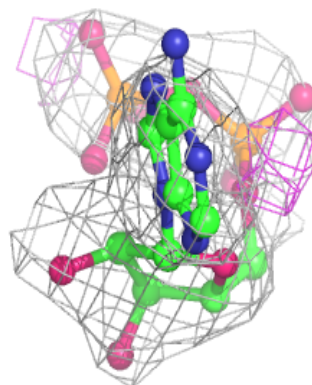
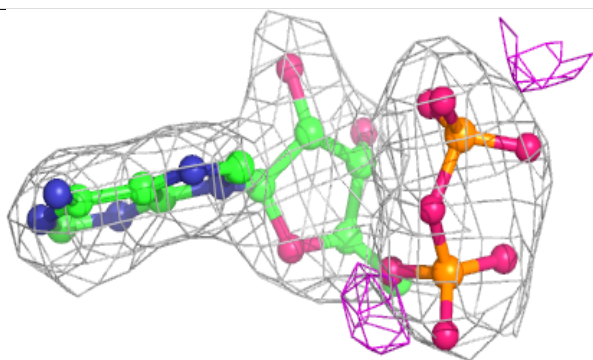
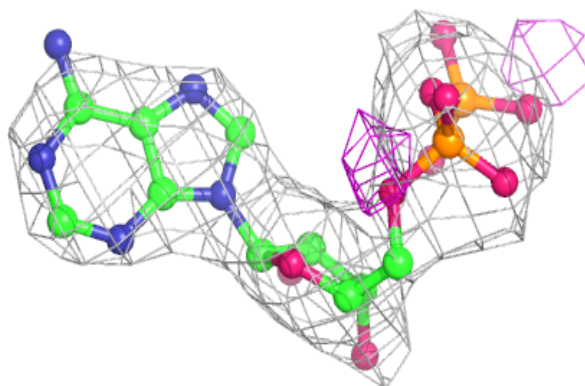


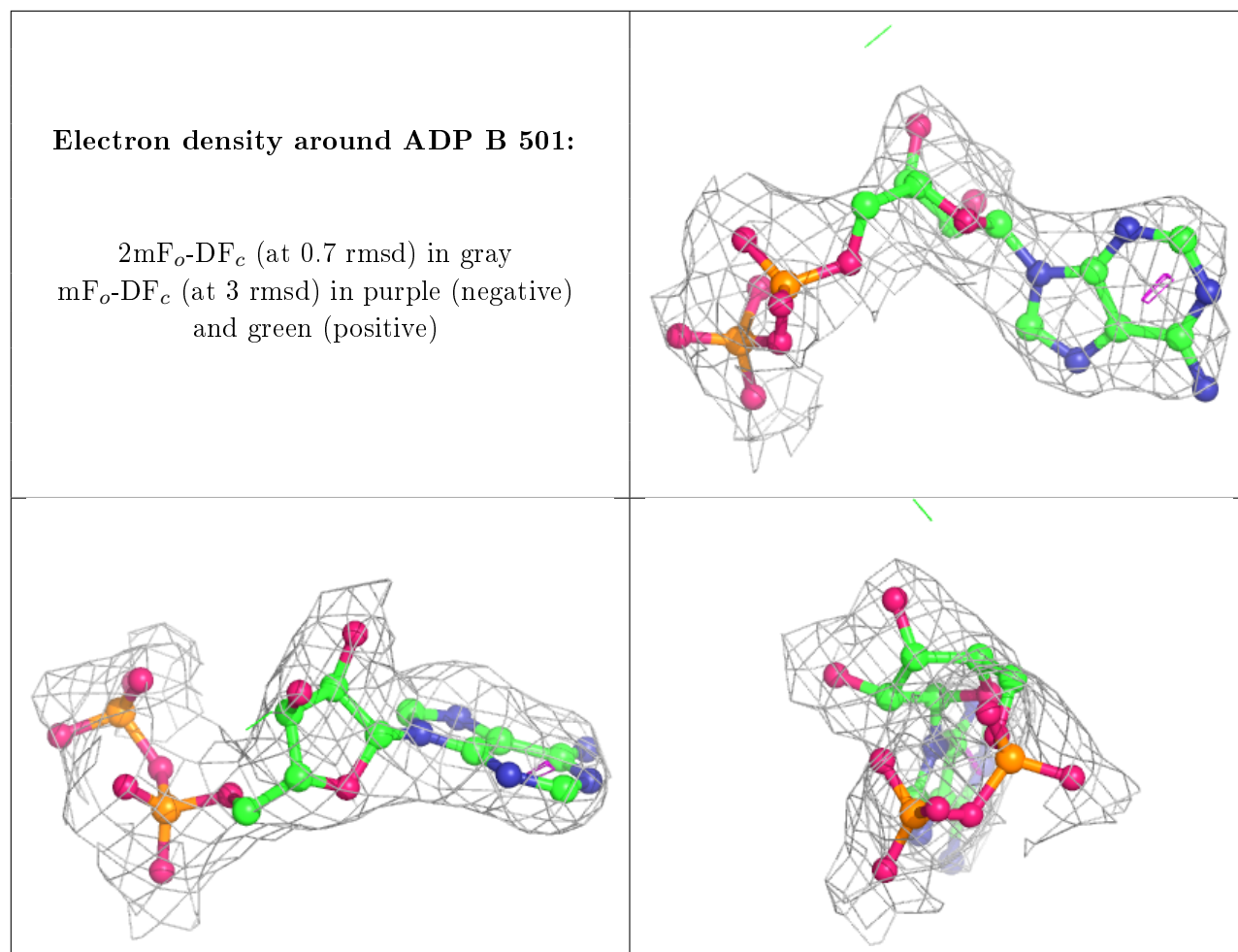
Electron density around ADP D 501:

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

**Electron density around ADP E 501:**

$2mF_o-DF_c$ (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.