



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:47 PM UTC

PDB ID : 6GJQ / pdb_00006gjQ
Title : human NBD1 of CFTR in complex with nanobody T27
Authors : Sigoillot, M.; Overtus, M.; Grodecka, M.; Scholl, D.; Garcia-Pino, A.; Laere-
mans, T.; He, L.; Pardon, E.; Hildebrandt, E.; Urbatsch, I.; Steyaert, J.;
Riordan, J.R.; Govaerts, C.
Deposited on : 2018-05-16
Resolution : 2.49 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:

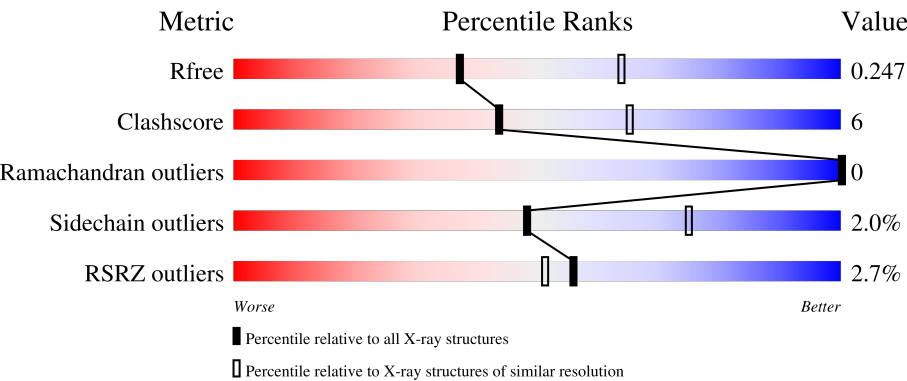
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.49 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	261	2% 60% 11% • 28%
1	C	261	% 62% 8% • 29%
1	E	261	2% 56% 14% • 28%
1	G	261	3% 62% 9% • 28%

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Mol	Chain	Length	Quality of chain
2	B	147	2% 72% 10% 18%
2	D	147	2% 69% 12% 18%
2	F	147	% 71% 11% 18%
2	H	147	3% 74% 8% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10035 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	0
			1450	932	231	277	10			
1	C	186	Total	C	N	O	S	0	0	0
			1444	928	231	275	10			
1	E	187	Total	C	N	O	S	0	0	0
			1453	933	235	275	10			
1	G	187	Total	C	N	O	S	0	0	0
			1445	926	233	276	10			

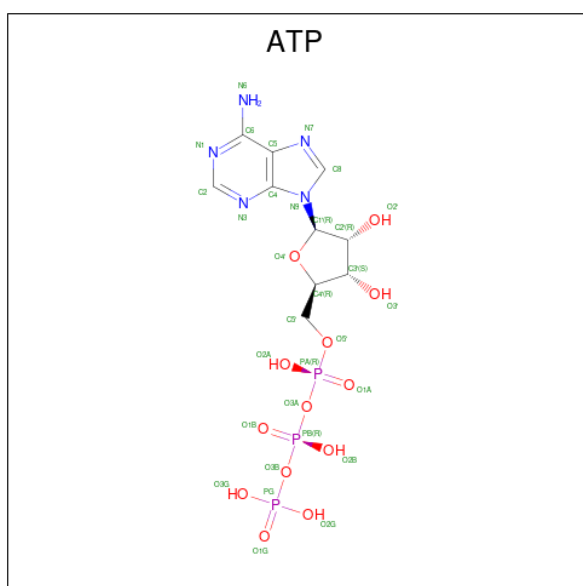
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	SER	-	expression tag	UNP Q20BJ8
A	492	PRO	SER	engineered mutation	UNP Q20BJ8
A	534	PRO	ALA	engineered mutation	UNP Q20BJ8
A	539	THR	ILE	engineered mutation	UNP Q20BJ8
C	386	SER	-	expression tag	UNP Q20BJ8
C	492	PRO	SER	engineered mutation	UNP Q20BJ8
C	534	PRO	ALA	engineered mutation	UNP Q20BJ8
C	539	THR	ILE	engineered mutation	UNP Q20BJ8
E	386	SER	-	expression tag	UNP Q20BJ8
E	492	PRO	SER	engineered mutation	UNP Q20BJ8
E	534	PRO	ALA	engineered mutation	UNP Q20BJ8
E	539	THR	ILE	engineered mutation	UNP Q20BJ8
G	386	SER	-	expression tag	UNP Q20BJ8
G	492	PRO	SER	engineered mutation	UNP Q20BJ8
G	534	PRO	ALA	engineered mutation	UNP Q20BJ8
G	539	THR	ILE	engineered mutation	UNP Q20BJ8

- Molecule 2 is a protein called Nanobody T27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			911	571	158	178	4			
2	D	121	Total	C	N	O	S	0	0	0
			923	577	161	181	4			
2	F	121	Total	C	N	O	S	0	0	0
			916	573	159	180	4			
2	H	121	Total	C	N	O	S	0	0	0
			920	575	160	181	4			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	46	Total	O	0	0
			46	46		

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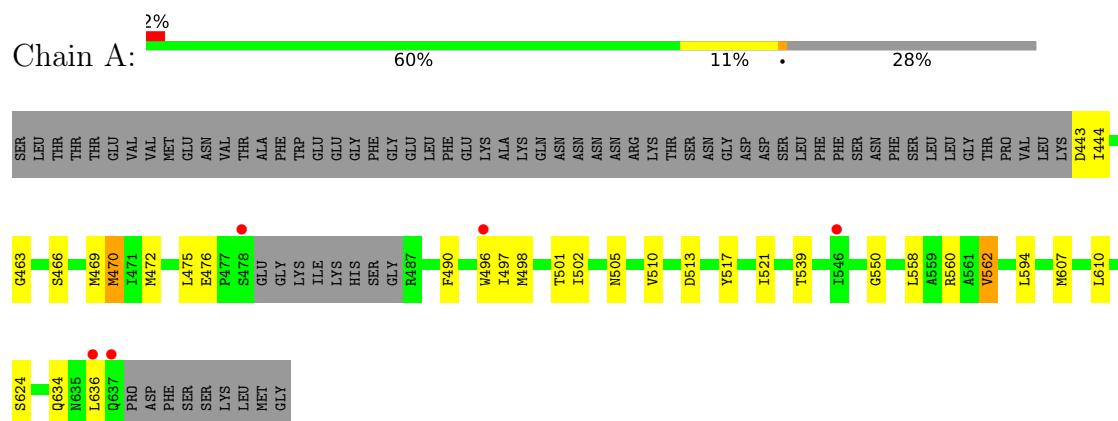
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	74	Total 74	O 74	0	0
4	D	34	Total 34	O 34	0	0
4	E	62	Total 62	O 62	0	0
4	F	44	Total 44	O 44	0	0
4	G	74	Total 74	O 74	0	0
4	H	44	Total 44	O 44	0	0

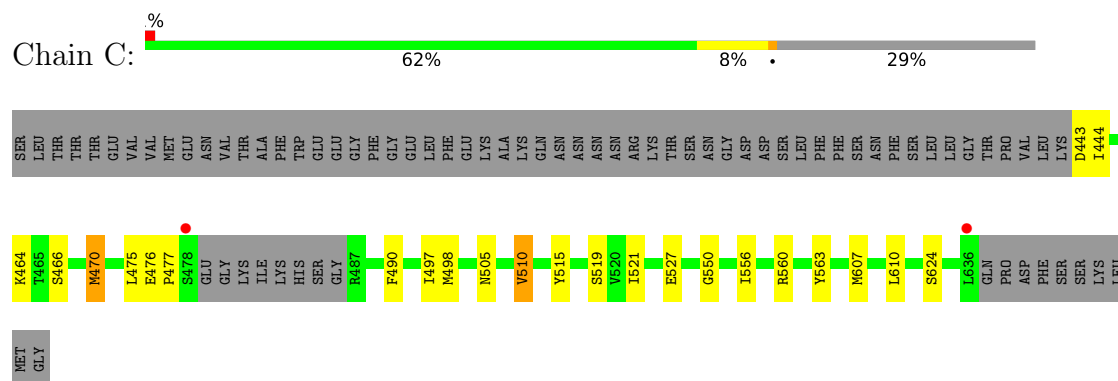
3 Residue-property plots [i](#)

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.

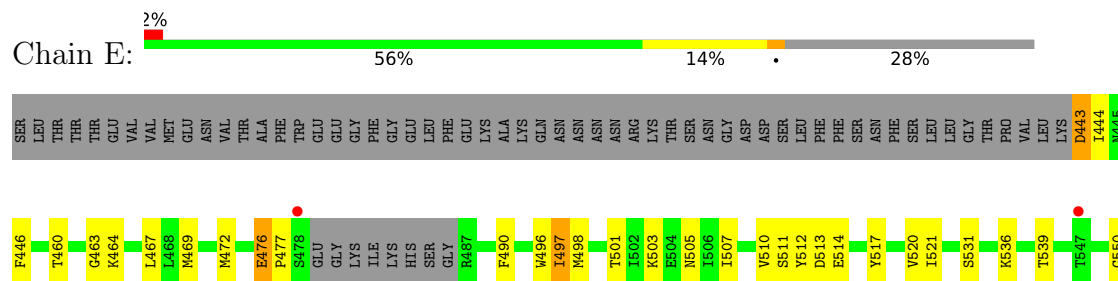
- Molecule 1: Cystic fibrosis transmembrane conductance regulator

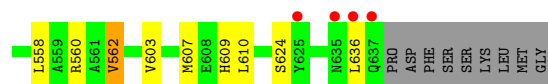


- Molecule 1: Cystic fibrosis transmembrane conductance regulator

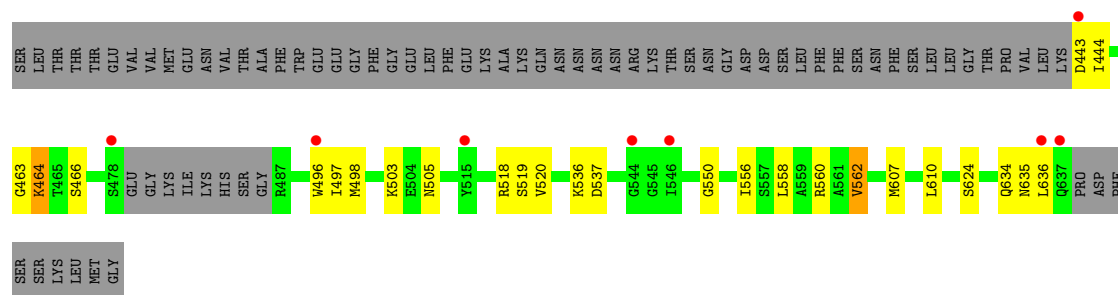


- Molecule 1: Cystic fibrosis transmembrane conductance regulator

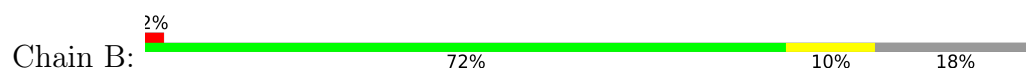




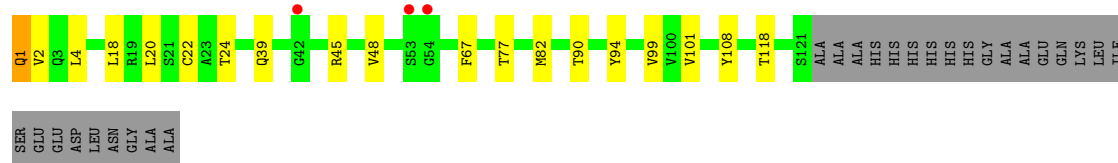
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



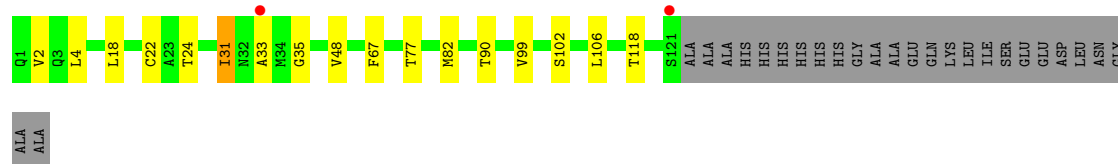
- Molecule 2: Nanobody T27



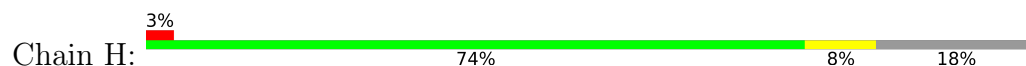
- Molecule 2: Nanobody T27



- Molecule 2: Nanobody T27



- Molecule 2: Nanobody T27





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.49Å 118.15Å 180.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.49 47.93 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.93-2.49) 99.3 (47.93-2.49)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.199 , 0.240 0.203 , 0.247	Depositor DCC
R_{free} test set	2434 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10035	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.51% 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: ATP

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	0.91	1/1474 (0.1%)	1.41	10/1983 (0.5%)
1	C	0.89	2/1468 (0.1%)	1.42	11/1975 (0.6%)
1	E	0.94	0/1477	1.44	17/1986 (0.9%)
1	G	0.89	0/1469	1.41	11/1977 (0.6%)
2	B	0.86	1/930 (0.1%)	1.21	3/1264 (0.2%)
2	D	0.82	0/942	1.19	2/1279 (0.2%)
2	F	0.87	2/935 (0.2%)	1.22	4/1270 (0.3%)
2	H	0.87	1/939 (0.1%)	1.20	2/1275 (0.2%)
All	All	0.89	7/9634 (0.1%)	1.34	60/13009 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	MET	SD-CE	-6.90	1.62	1.79
1	C	497	ILE	C-O	-5.81	1.18	1.23
1	C	470	MET	SD-CE	-5.64	1.65	1.79
2	H	82	MET	SD-CE	-5.54	1.65	1.79
2	F	82	MET	SD-CE	-5.39	1.66	1.79
2	B	82	MET	SD-CE	-5.34	1.66	1.79
2	F	31	ILE	C-O	-5.24	1.18	1.24

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	443	ASP	CA-CB-CG	9.95	122.55	112.60
2	F	33	ALA	N-CA-C	8.03	122.32	111.24
2	D	48	VAL	N-CA-C	-7.42	104.51	111.48
2	F	48	VAL	N-CA-C	-7.30	104.62	111.48
1	G	464	LYS	N-CA-C	7.15	118.72	111.07
2	B	48	VAL	N-CA-C	-7.11	104.80	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	443	ASP	CA-CB-CG	7.08	119.68	112.60
2	H	48	VAL	N-CA-C	-6.99	104.91	111.48
1	E	513	ASP	CA-C-N	6.85	129.79	120.54
1	E	513	ASP	C-N-CA	6.85	129.79	120.54
1	G	607	MET	CA-C-N	6.58	129.10	120.28
1	G	607	MET	C-N-CA	6.58	129.10	120.28
1	G	519	SER	CA-C-N	6.36	128.57	120.56
1	G	519	SER	C-N-CA	6.36	128.57	120.56
1	C	607	MET	CA-C-N	6.26	128.67	120.28
1	C	607	MET	C-N-CA	6.26	128.67	120.28
2	B	51	PHE	N-CA-C	-6.26	99.07	109.46
1	G	518	ARG	CA-C-N	6.22	128.52	120.44
1	G	518	ARG	C-N-CA	6.22	128.52	120.44
1	E	476	GLU	CB-CG-CD	6.13	123.02	112.60
1	A	513	ASP	CA-CB-CG	6.06	118.66	112.60
2	F	35	GLY	N-CA-C	6.02	122.53	110.97
1	A	607	MET	CA-C-N	6.00	128.91	120.28
1	A	607	MET	C-N-CA	6.00	128.91	120.28
1	G	610	LEU	CA-C-N	6.00	128.91	120.28
1	G	610	LEU	C-N-CA	6.00	128.91	120.28
1	E	490	PHE	CA-CB-CG	5.99	119.79	113.80
1	E	609	HIS	CA-C-N	5.98	128.89	120.28
1	E	609	HIS	C-N-CA	5.98	128.89	120.28
1	E	514	GLU	CA-C-N	5.87	128.43	120.44
1	E	514	GLU	C-N-CA	5.87	128.43	120.44
1	C	610	LEU	CA-C-N	5.87	128.73	120.28
1	C	610	LEU	C-N-CA	5.87	128.73	120.28
1	A	610	LEU	CA-C-N	5.81	128.64	120.28
1	A	610	LEU	C-N-CA	5.81	128.64	120.28
1	E	610	LEU	CA-C-N	5.78	128.61	120.28
1	E	610	LEU	C-N-CA	5.78	128.61	120.28
2	D	67	PHE	CA-CB-CG	5.71	119.51	113.80
1	E	607	MET	CA-C-N	5.70	127.91	120.28
1	E	607	MET	C-N-CA	5.70	127.91	120.28
1	C	490	PHE	CA-CB-CG	5.54	119.34	113.80
2	B	67	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	550	GLY	CA-C-N	5.46	126.01	120.00
1	A	550	GLY	C-N-CA	5.46	126.01	120.00
2	H	67	PHE	CA-CB-CG	5.40	119.20	113.80
1	G	550	GLY	CA-C-N	5.39	125.93	120.00
1	G	550	GLY	C-N-CA	5.39	125.93	120.00
1	A	502	ILE	CA-C-N	5.24	127.25	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	ILE	C-N-CA	5.24	127.25	120.44
1	C	556	ILE	CB-CA-C	-5.20	105.04	112.22
1	C	519	SER	CA-C-N	5.17	127.07	120.56
1	C	519	SER	C-N-CA	5.17	127.07	120.56
1	A	490	PHE	CA-CB-CG	5.08	118.88	113.80
2	F	67	PHE	CA-CB-CG	5.05	118.85	113.80
1	E	550	GLY	CA-C-N	5.04	125.55	120.00
1	E	550	GLY	C-N-CA	5.04	125.55	120.00
1	E	507	ILE	CA-C-N	5.04	129.98	122.82
1	E	507	ILE	C-N-CA	5.04	129.98	122.82
1	C	550	GLY	CA-C-N	5.03	125.53	120.00
1	C	550	GLY	C-N-CA	5.03	125.53	120.00

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	1450	0	1447	32	0
1	C	1444	0	1445	15	0
1	E	1453	0	1459	36	0
1	G	1445	0	1439	13	0
2	B	911	0	856	6	0
2	D	923	0	874	18	0
2	F	916	0	865	5	0
2	H	920	0	871	5	0
3	A	31	0	12	4	0
3	C	31	0	12	3	0
3	E	31	0	12	4	0
3	G	31	0	12	5	0
4	A	71	0	0	0	0
4	B	46	0	0	0	0
4	C	74	0	0	0	0
4	D	34	0	0	0	0
4	E	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	44	0	0	0	0
4	G	74	0	0	0	0
4	H	44	0	0	0	0
All	All	10035	0	9304	115	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 6.

All (115) 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:E:463:GLY:HA2	3:E:701:ATP:H5'2	1.34	1.10
1:G:463:GLY:HA2	3:G:701:ATP:H5'2	1.39	1.01
2:D:18:LEU:HB3	2:D:82:MET:HE3	1.44	0.99
2:D:1:GLN:HE21	2:D:1:GLN:HA	1.30	0.93
1:A:469:MET:HG3	1:E:472:MET:HE1	1.50	0.92
1:E:463:GLY:HA2	3:E:701:ATP:C5'	2.03	0.87
1:C:466:SER:HB2	3:C:701:ATP:H5'2	1.56	0.85
1:A:472:MET:HE1	1:E:469:MET:HG3	1.64	0.80
1:A:463:GLY:HA2	3:A:701:ATP:H5'2	1.64	0.80
2:D:1:GLN:HA	2:D:1:GLN:NE2	1.95	0.78
2:D:18:LEU:HD23	2:D:82:MET:HE1	1.69	0.75
1:G:635:ASN:O	1:G:636:LEU:HD23	1.88	0.74
2:D:18:LEU:HD23	2:D:82:MET:CE	2.18	0.73
1:E:463:GLY:CA	3:E:701:ATP:H5'2	2.19	0.71
1:E:460:THR:HG23	3:E:701:ATP:O1G	1.91	0.70
2:H:4:LEU:HD22	2:H:24:THR:HG22	1.74	0.69
2:D:4:LEU:HD22	2:D:24:THR:HG22	1.76	0.68
1:E:510:VAL:HG12	1:E:511:SER:N	2.09	0.68
2:F:4:LEU:HD22	2:F:24:THR:HG22	1.77	0.67
1:C:466:SER:HB2	3:C:701:ATP:C5'	2.23	0.67
2:B:4:LEU:HD22	2:B:24:THR:HG22	1.78	0.66
1:E:510:VAL:CG1	1:E:511:SER:N	2.59	0.66
1:G:444:ILE:HG23	1:G:624:SER:HB2	1.79	0.65
1:C:466:SER:CB	3:C:701:ATP:H5'2	2.27	0.63
1:E:444:ILE:HG23	1:E:624:SER:HB2	1.81	0.63
1:G:634:GLN:C	1:G:636:LEU:H	2.07	0.63
2:D:18:LEU:CB	2:D:82:MET:HE3	2.25	0.62
1:C:444:ILE:HG23	1:C:624:SER:HB2	1.82	0.62
1:A:476:GLU:OE2	1:E:496:TRP:HH2	1.82	0.62
1:A:444:ILE:HG23	1:A:624:SER:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:MET:HE3	1:E:472:MET:HE3	1.80	0.61
1:A:496:TRP:HH2	1:E:476:GLU:CD	2.09	0.60
1:A:505:ASN:O	1:A:560:ARG:HD3	2.01	0.60
1:A:496:TRP:CZ3	1:E:443:ASP:HB3	2.38	0.59
2:D:18:LEU:HB3	2:D:82:MET:CE	2.26	0.59
2:D:2:VAL:HG21	2:D:99:VAL:HG11	1.84	0.58
1:A:466:SER:HB2	3:A:701:ATP:H5'1	1.85	0.58
2:D:2:VAL:HG11	2:D:99:VAL:HG21	1.86	0.57
1:E:505:ASN:O	1:E:560:ARG:HD3	2.04	0.57
1:C:505:ASN:O	1:C:560:ARG:HD3	2.05	0.56
1:A:496:TRP:CH2	1:E:443:ASP:HB3	2.41	0.55
1:E:469:MET:HA	1:E:472:MET:HE2	1.88	0.55
1:E:503:LYS:HE2	1:E:512:TYR:CE1	2.42	0.55
1:E:531:SER:HA	1:E:536:LYS:HD3	1.87	0.55
1:E:464:LYS:HD2	1:E:603:VAL:HG13	1.89	0.54
1:A:517:TYR:O	1:A:521:ILE:HG12	2.08	0.54
1:A:470:MET:CE	1:A:475:LEU:HD12	2.38	0.54
1:C:470:MET:HE1	1:C:475:LEU:HD12	1.90	0.54
1:A:496:TRP:HH2	1:E:476:GLU:OE2	1.91	0.53
1:C:470:MET:CE	1:C:475:LEU:HD12	2.39	0.53
1:E:496:TRP:C	1:E:497:ILE:HG12	2.33	0.53
1:C:510:VAL:HG22	1:C:563:TYR:HE2	1.74	0.52
1:A:476:GLU:OE2	1:E:496:TRP:CH2	2.63	0.52
2:D:1:GLN:NE2	2:D:1:GLN:CA	2.71	0.52
1:A:496:TRP:CH2	1:E:476:GLU:OE2	2.64	0.51
1:A:470:MET:HE1	1:A:475:LEU:CD1	2.40	0.51
1:C:470:MET:HE1	1:C:475:LEU:CD1	2.41	0.50
1:A:443:ASP:HA	1:E:496:TRP:CH2	2.45	0.50
1:G:505:ASN:O	1:G:560:ARG:HD3	2.10	0.50
2:D:39:GLN:HB3	2:D:45:ARG:HA	1.94	0.50
1:G:464:LYS:HE3	3:G:701:ATP:O2B	2.11	0.50
1:C:510:VAL:HG22	1:C:563:TYR:CE2	2.46	0.49
1:A:470:MET:HE2	1:E:496:TRP:CE3	2.47	0.49
1:E:446:PHE:CE1	1:E:476:GLU:HG3	2.47	0.49
2:B:2:VAL:HG11	2:B:99:VAL:HG21	1.94	0.48
2:F:102:SER:HB3	2:F:106:LEU:HB2	1.96	0.47
2:B:39:GLN:HB3	2:B:45:ARG:HA	1.95	0.47
1:E:476:GLU:HG3	1:E:477:PRO:HA	1.95	0.47
2:H:39:GLN:HB3	2:H:45:ARG:HA	1.97	0.47
1:A:470:MET:CE	1:A:475:LEU:CD1	2.93	0.46
1:G:558:LEU:O	1:G:562:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:TRP:HD1	1:A:560:ARG:CZ	2.28	0.46
1:C:498:MET:HE2	1:C:498:MET:HB3	1.89	0.46
1:A:558:LEU:O	1:A:562:VAL:HG13	2.15	0.46
1:A:463:GLY:HA2	3:A:701:ATP:C5'	2.41	0.46
2:D:39:GLN:HG2	2:D:94:TYR:HE2	1.80	0.45
2:D:101:VAL:HG11	2:D:108:TYR:HB2	1.98	0.45
1:E:496:TRP:HD1	1:E:560:ARG:CZ	2.30	0.45
1:E:517:TYR:O	1:E:521:ILE:HG12	2.17	0.45
1:A:634:GLN:C	1:A:636:LEU:H	2.25	0.45
2:B:39:GLN:HG2	2:B:94:TYR:HE1	1.81	0.45
2:D:20:LEU:HG	2:D:82:MET:HE2	1.99	0.45
2:D:18:LEU:HD23	2:D:82:MET:HE3	1.96	0.44
2:F:22:CYS:O	2:F:77:THR:HG23	2.17	0.44
2:F:90:THR:HG23	2:F:118:THR:HA	1.99	0.44
1:A:470:MET:HE3	1:A:475:LEU:HD12	2.00	0.44
1:E:558:LEU:O	1:E:562:VAL:HG13	2.17	0.44
1:G:466:SER:HB2	3:G:701:ATP:H5'1	2.00	0.44
1:A:496:TRP:HD1	1:A:560:ARG:NH2	2.15	0.44
1:A:594:LEU:HD11	1:C:515:TYR:HB3	2.00	0.44
1:E:467:LEU:HD11	1:E:476:GLU:HG2	2.00	0.44
1:A:466:SER:HB2	3:A:701:ATP:C5'	2.48	0.44
1:E:496:TRP:HD1	1:E:560:ARG:NH2	2.16	0.44
1:G:496:TRP:HD1	1:G:560:ARG:NH2	2.15	0.43
1:G:520:VAL:HG22	1:G:562:VAL:HG23	1.99	0.43
2:D:90:THR:HG23	2:D:118:THR:HA	2.00	0.43
1:G:496:TRP:HD1	1:G:560:ARG:CZ	2.31	0.43
2:H:90:THR:HG23	2:H:118:THR:HA	2.00	0.43
1:G:443:ASP:OD2	3:G:701:ATP:N6	2.52	0.42
2:H:39:GLN:HG2	2:H:94:TYR:HE1	1.83	0.42
1:A:472:MET:HB3	1:E:472:MET:HB3	2.01	0.42
1:G:466:SER:CB	3:G:701:ATP:H5'1	2.50	0.42
2:B:90:THR:HG23	2:B:118:THR:HA	2.02	0.42
1:C:476:GLU:HG3	1:C:477:PRO:HA	2.00	0.42
1:A:501:THR:HA	1:A:539:THR:O	2.20	0.42
1:C:521:ILE:HG22	1:C:527:GLU:HG2	2.00	0.42
2:D:22:CYS:O	2:D:77:THR:HG23	2.20	0.42
2:H:51:PHE:CE2	2:H:71:ARG:HB2	2.56	0.41
1:C:470:MET:CE	1:C:475:LEU:CD1	2.99	0.41
1:E:501:THR:HA	1:E:539:THR:O	2.20	0.41
1:A:476:GLU:CD	1:E:496:TRP:HH2	2.28	0.41
2:F:2:VAL:HG11	2:F:99:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:CYS:O	2:B:77:THR:HG23	2.21	0.40
1:A:470:MET:HE1	1:A:475:LEU:HD12	1.99	0.40
1:E:520:VAL:HG22	1:E:562:VAL:HG23	2.03	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	183/261 (70%)	173 (94%)	10 (6%)	0	100	100
1	C	182/261 (70%)	176 (97%)	6 (3%)	0	100	100
1	E	183/261 (70%)	176 (96%)	7 (4%)	0	100	100
1	G	183/261 (70%)	176 (96%)	7 (4%)	0	100	100
2	B	119/147 (81%)	117 (98%)	2 (2%)	0	100	100
2	D	119/147 (81%)	117 (98%)	2 (2%)	0	100	100
2	F	119/147 (81%)	118 (99%)	1 (1%)	0	100	100
2	H	119/147 (81%)	118 (99%)	1 (1%)	0	100	100
All	All	1207/1632 (74%)	1171 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/227 (69%)	152 (97%)	4 (3%)	40	68
1	C	156/227 (69%)	154 (99%)	2 (1%)	61	82
1	E	157/227 (69%)	153 (98%)	4 (2%)	42	69
1	G	156/227 (69%)	149 (96%)	7 (4%)	24	49
2	B	92/114 (81%)	92 (100%)	0	100	100
2	D	95/114 (83%)	94 (99%)	1 (1%)	65	84
2	F	94/114 (82%)	92 (98%)	2 (2%)	47	74
2	H	95/114 (83%)	95 (100%)	0	100	100
All	All	1001/1364 (73%)	981 (98%)	20 (2%)	48	75

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	497	ILE
1	A	498	MET
1	A	510	VAL
1	A	562	VAL
1	C	464	LYS
1	C	510	VAL
2	D	1	GLN
1	E	497	ILE
1	E	498	MET
1	E	562	VAL
1	E	636	LEU
2	F	18	LEU
2	F	31	ILE
1	G	497	ILE
1	G	498	MET
1	G	503	LYS
1	G	536	LYS
1	G	537	ASP
1	G	556	ILE
1	G	562	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	635	ASN
2	B	5	GLN

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Mol	Chain	Res	Type
2	B	58	ASN
2	B	73	ASN
2	D	1	GLN
2	D	58	ASN
2	D	73	ASN
1	E	452	GLN
1	E	525	GLN
2	F	5	GLN
2	F	58	ASN
2	F	73	ASN
2	F	81	GLN
1	G	525	GLN
2	H	58	ASN
2	H	73	ASN
2	H	81	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	ATP	A	701	-	32,33,33	1.62	6 (18%)	48,52,52	2.11	13 (27%)
3	ATP	C	701	-	32,33,33	0.67	1 (3%)	48,52,52	0.82	0
3	ATP	E	701	-	32,33,33	0.86	1 (3%)	48,52,52	0.77	1 (2%)
3	ATP	G	701	-	32,33,33	0.78	2 (6%)	48,52,52	0.85	2 (4%)

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	ATP	A	701	-	-	10/22/38/38	0/3/3/3
3	ATP	C	701	-	-	8/22/38/38	0/3/3/3
3	ATP	E	701	-	-	5/22/38/38	0/3/3/3
3	ATP	G	701	-	-	6/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ATP	C5-C4	5.32	1.48	1.39
3	A	701	ATP	C5-C6	3.44	1.50	1.41
3	E	701	ATP	PA-O5'	3.43	1.72	1.59
3	G	701	ATP	PG-O1G	2.59	1.58	1.50
3	G	701	ATP	PA-O5'	2.56	1.69	1.59
3	A	701	ATP	C8-N7	2.47	1.36	1.31
3	C	701	ATP	PA-O5'	2.46	1.69	1.59
3	A	701	ATP	PA-O3A	2.38	1.62	1.59
3	A	701	ATP	C5-N7	-2.31	1.34	1.39
3	A	701	ATP	PB-O2B	-2.13	1.45	1.55

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ATP	C5-C4-N3	-7.00	117.08	126.72
3	A	701	ATP	C4-C5-N7	-5.03	104.83	110.58
3	A	701	ATP	C2-N3-C4	4.43	122.65	111.83
3	A	701	ATP	N3-C4-N9	4.41	134.67	127.17
3	A	701	ATP	N3-C2-N1	-3.92	122.65	128.58
3	A	701	ATP	O4'-C1'-N9	3.12	114.08	108.09
3	A	701	ATP	C5-N7-C8	3.10	108.33	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ATP	O5'-C5'-C4'	3.10	119.54	108.99
3	A	701	ATP	C6-C5-N7	3.09	138.05	132.09
3	G	701	ATP	O5'-C5'-C4'	3.04	119.35	108.99
3	E	701	ATP	O5'-C5'-C4'	2.59	117.80	108.99
3	A	701	ATP	C2-N1-C6	2.31	122.53	118.73
3	A	701	ATP	C5-C4-N9	2.23	108.24	105.81
3	A	701	ATP	C2'-C3'-C4'	2.10	106.67	102.61
3	G	701	ATP	O5'-PA-O1A	2.02	116.95	108.94
3	A	701	ATP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	ATP	PB-O3B-PG-O2G
3	A	701	ATP	C5'-O5'-PA-O1A
3	A	701	ATP	C5'-O5'-PA-O2A
3	A	701	ATP	C5'-O5'-PA-O3A
3	C	701	ATP	C5'-O5'-PA-O1A
3	C	701	ATP	C5'-O5'-PA-O2A
3	C	701	ATP	C5'-O5'-PA-O3A
3	G	701	ATP	C5'-O5'-PA-O1A
3	G	701	ATP	C5'-O5'-PA-O2A
3	G	701	ATP	C5'-O5'-PA-O3A
3	A	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	C3'-C4'-C5'-O5'
3	C	701	ATP	C3'-C4'-C5'-O5'
3	C	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	PB-O3B-PG-O3G
3	G	701	ATP	PA-O3A-PB-O1B
3	E	701	ATP	C5'-O5'-PA-O2A
3	C	701	ATP	PA-O3A-PB-O2B
3	E	701	ATP	PG-O3B-PB-O2B
3	E	701	ATP	PA-O3A-PB-O2B
3	A	701	ATP	PA-O3A-PB-O1B
3	C	701	ATP	PG-O3B-PB-O2B
3	G	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	PB-O3B-PG-O1G
3	C	701	ATP	PA-O3A-PB-O1B
3	E	701	ATP	PG-O3B-PB-O1B
3	E	701	ATP	PA-O3A-PB-O1B
3	A	701	ATP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	G	701	ATP	PA-O3A-PB-O2B

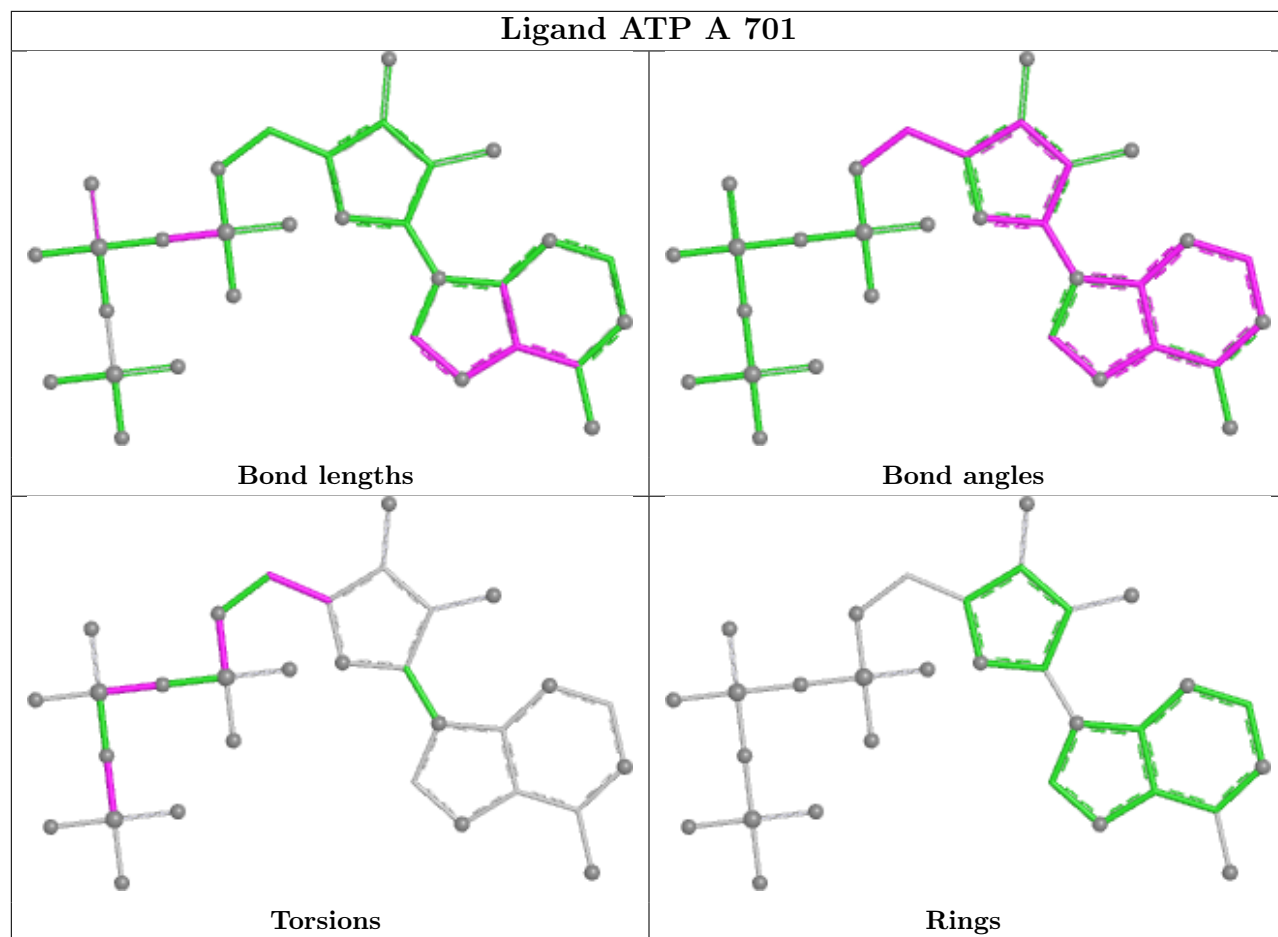
There are no ring outliers.

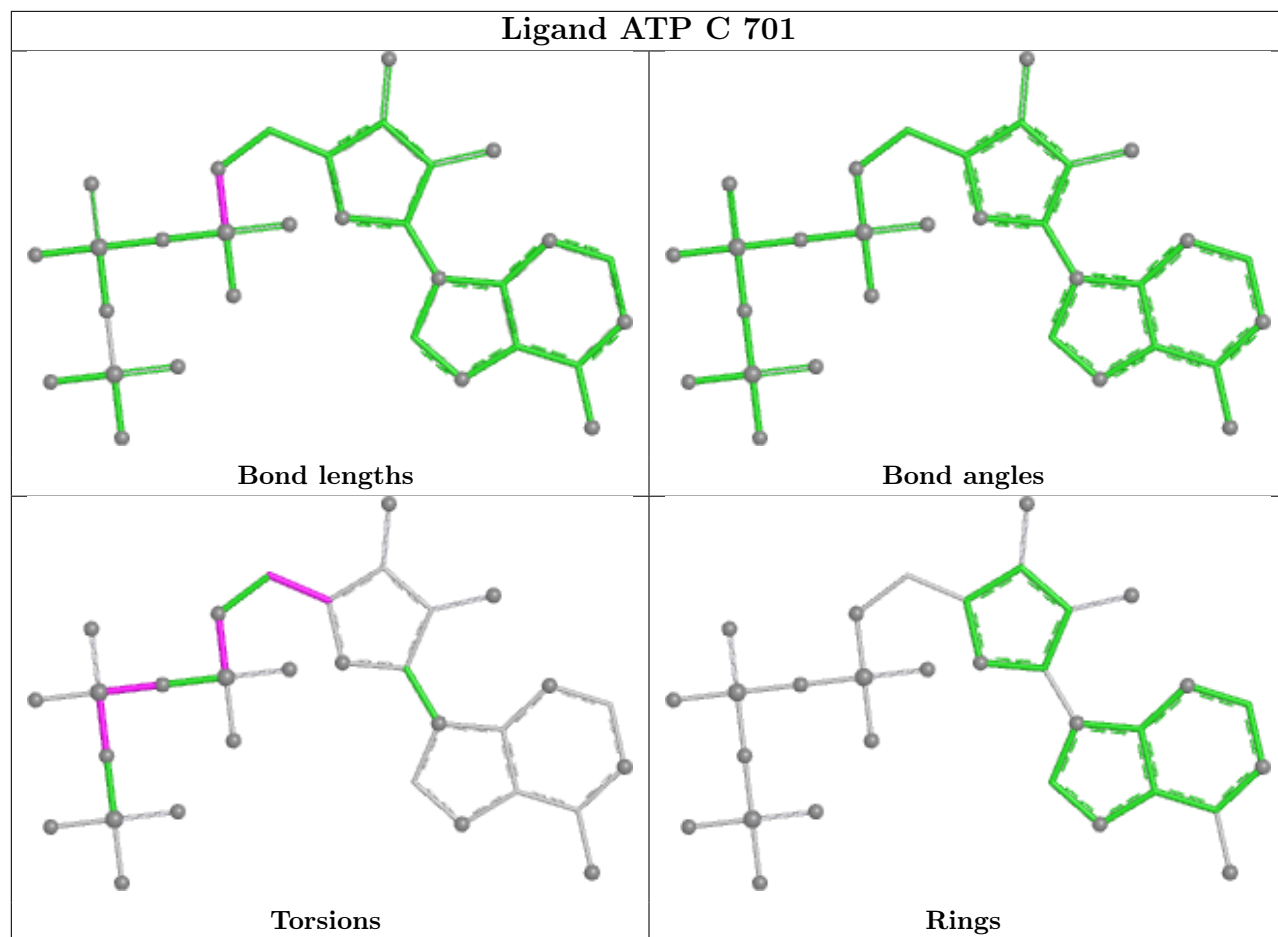
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	ATP	4	0
3	C	701	ATP	3	0
3	E	701	ATP	4	0
3	G	701	ATP	5	0

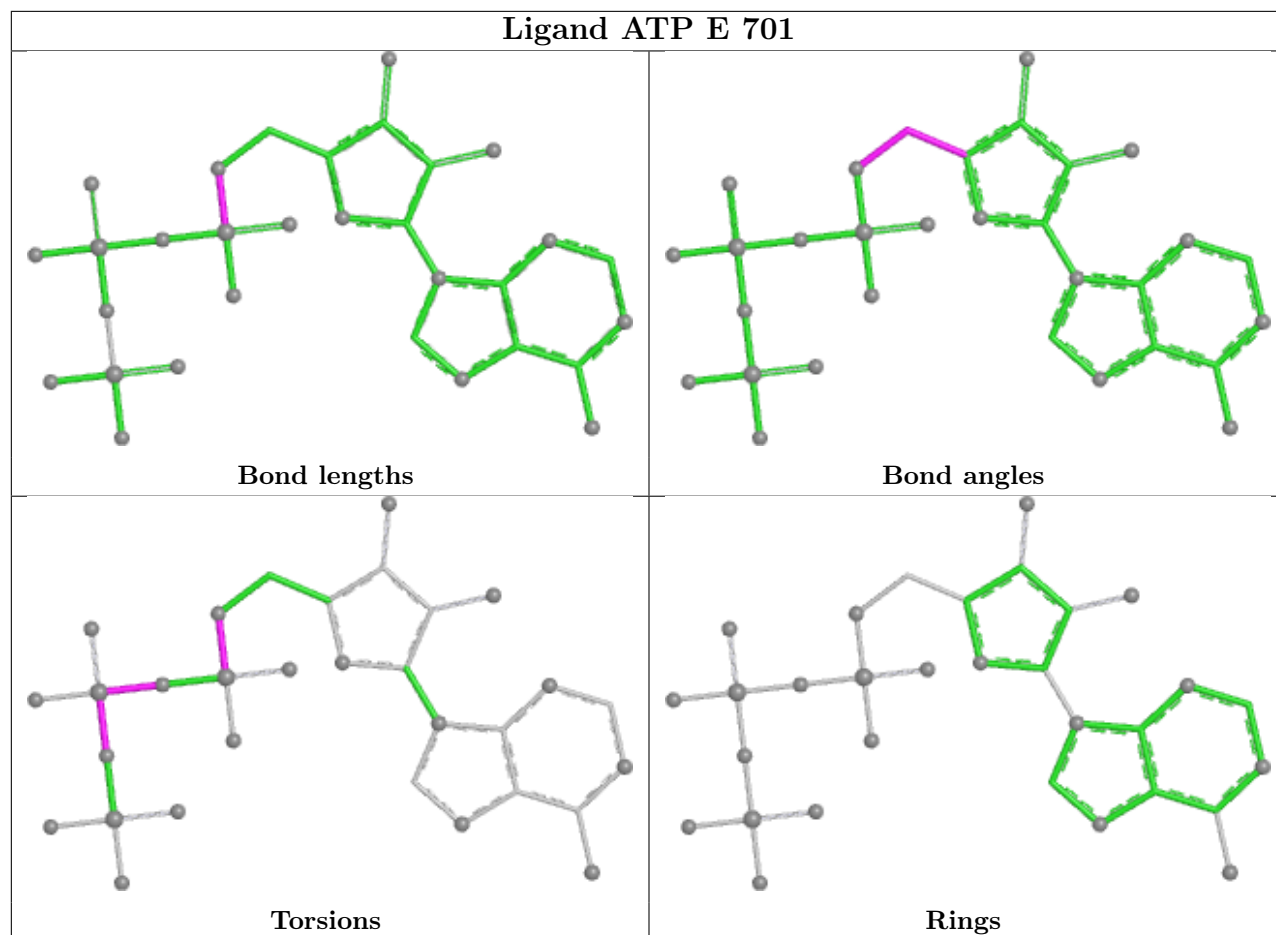
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

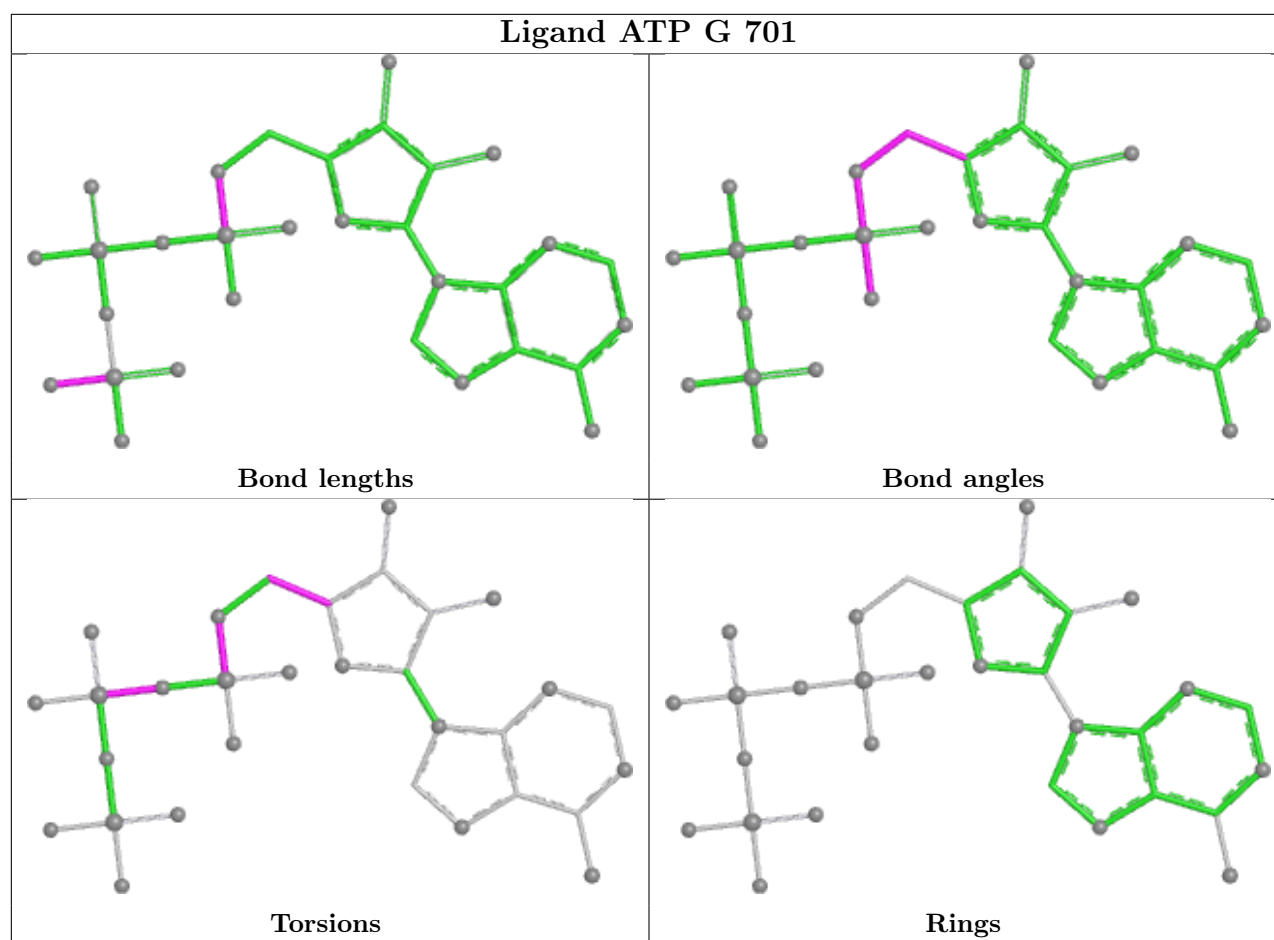
Ligand ATP A 701





Ligand ATP E 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	187/261 (71%)	0.04	5 (2%) 56 51	34, 47, 76, 98	0
1	C	186/261 (71%)	-0.05	2 (1%) 78 75	34, 47, 72, 91	0
1	E	187/261 (71%)	0.19	6 (3%) 50 46	36, 48, 79, 127	0
1	G	187/261 (71%)	0.07	8 (4%) 40 35	30, 47, 75, 102	0
2	B	121/147 (82%)	0.01	3 (2%) 58 54	34, 49, 70, 91	0
2	D	121/147 (82%)	0.13	3 (2%) 58 54	34, 51, 73, 90	0
2	F	121/147 (82%)	0.11	2 (1%) 69 65	35, 48, 69, 80	0
2	H	121/147 (82%)	0.07	4 (3%) 49 45	32, 47, 68, 85	0
All	All	1231/1632 (75%)	0.07	33 (2%) 56 51	30, 48, 75, 127	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	478	SER	5.0
1	E	636	LEU	4.7
1	G	515	TYR	4.5
1	C	478	SER	3.7
2	B	53	SER	3.5
1	G	546	ILE	3.4
1	G	637	GLN	3.3
1	A	478	SER	3.2
2	D	53	SER	3.2
2	B	121	SER	3.2
1	G	636	LEU	2.9
1	A	637	GLN	2.9
1	E	637	GLN	2.9
1	G	544	GLY	2.8
1	G	478	SER	2.8
2	D	54	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	108	TYR	2.5
1	C	636	LEU	2.5
1	G	496	TRP	2.4
1	A	546	ILE	2.4
2	H	113	GLN	2.4
1	E	625	TYR	2.4
1	E	635	ASN	2.4
1	A	496	TRP	2.3
2	F	33	ALA	2.3
1	A	636	LEU	2.2
2	H	53	SER	2.2
2	H	121	SER	2.2
1	E	547	THR	2.1
2	D	42	GLY	2.1
1	G	443	ASP	2.1
2	B	1	GLN	2.1
2	F	121	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

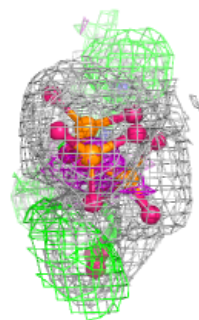
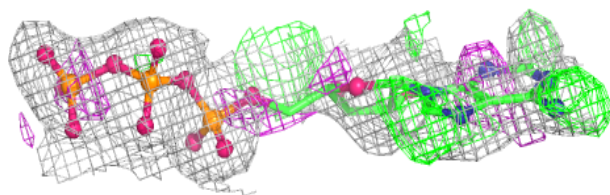
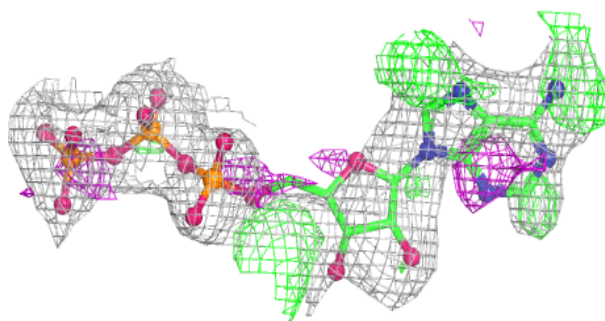
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	A	701	31/31	0.79	0.20	52,99,109,111	0
3	ATP	C	701	31/31	0.80	0.18	42,84,95,99	0
3	ATP	G	701	31/31	0.80	0.20	44,93,101,102	0
3	ATP	E	701	31/31	0.83	0.20	39,92,99,102	0

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.

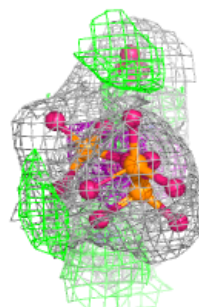
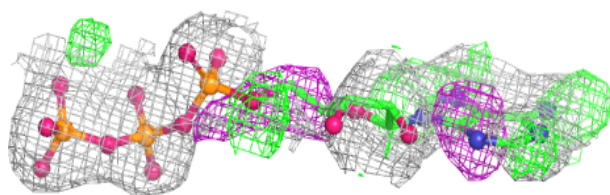
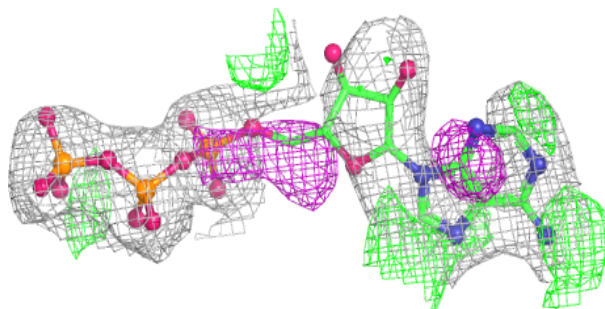
Electron density around ATP A 701:

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

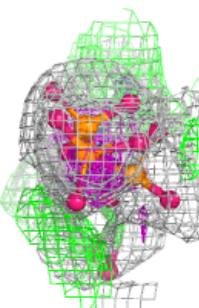
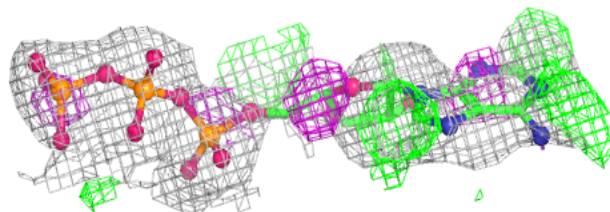
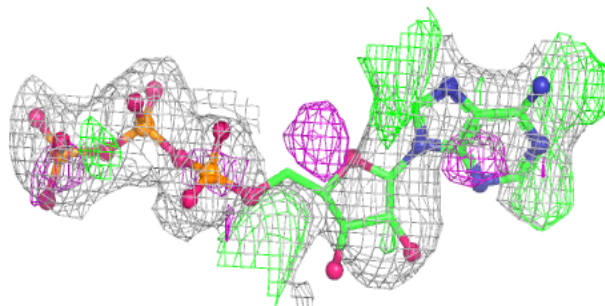


Electron density around ATP C 701:

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

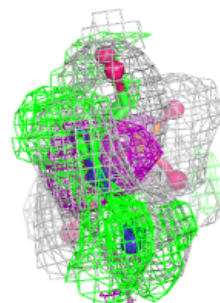
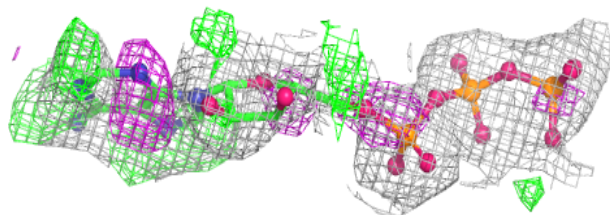
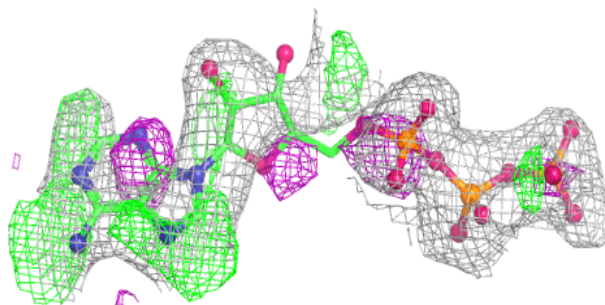
**Electron density around ATP G 701:**

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



Electron density around ATP E 701:

$2mF_o - DF_c$ (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.