Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 09:20 PM EDT

PDB ID	:	1NBM
Title	:	THE STRUCTURE OF BOVINE F1-ATPASE COVALENTLY INHIBITED WITH 4-CHLORO-7-NITROBENZOFURAZAN
Authors	:	Orriss, G.L.; Leslie, A.G.W.; Braig, K.; Walker, J.E.
Deposited on	:	1998-04-30
Resolution	:	3.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

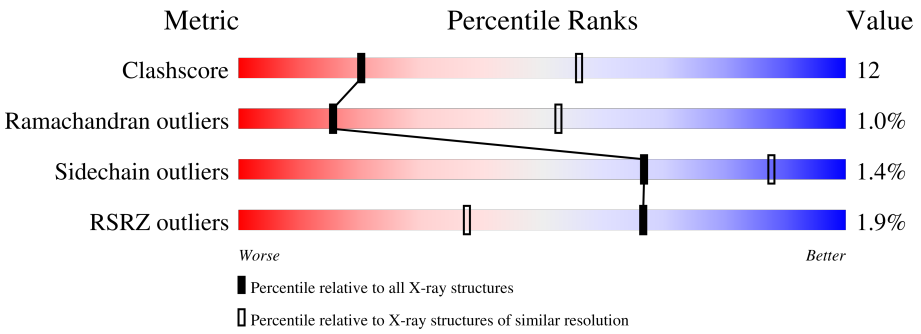
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	510	.% 69% 26% • 5%
1	B	510	2% 64% 31% • 5%
1	C	510	.% 69% 27% •
2	D	480	.% 68% 28% • •
2	F	480	68% 29% •
3	E	480	.% 69% 27% • •

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Mol	Chain	Length	Quality of chain
4	G	272	8% 33% 12% 55%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 23057 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 F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3715	2341	656	706	12	0	0	0
1	B	487	3715	2341	656	706	12	59	0	0
1	C	492	3748	2360	661	715	12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

- Molecule 2 is a protein called F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	467	3539	2243	601	684	11	0	0	0
2	F	466	3530	2238	600	681	11	0	0	0

- Molecule 3 is a protein called F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	466	3540	2244	603	682	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	311	TYN	TYR	modified residue	UNP P00829

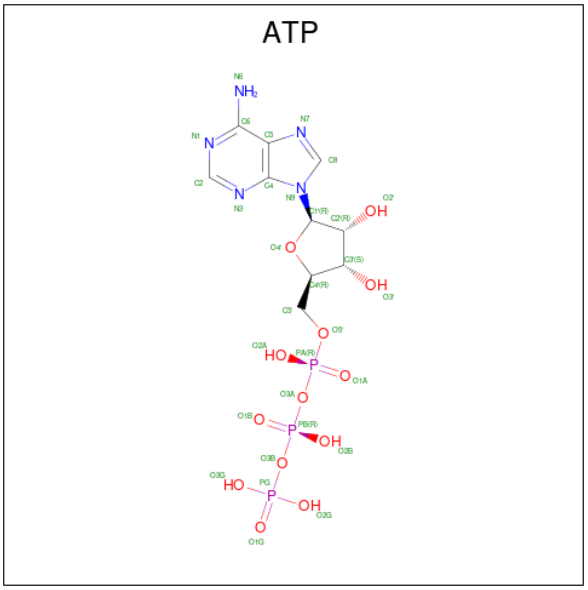
- Molecule 4 is a protein called F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	122	945	591	171	176	7	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0
5	F	1	1	1	0	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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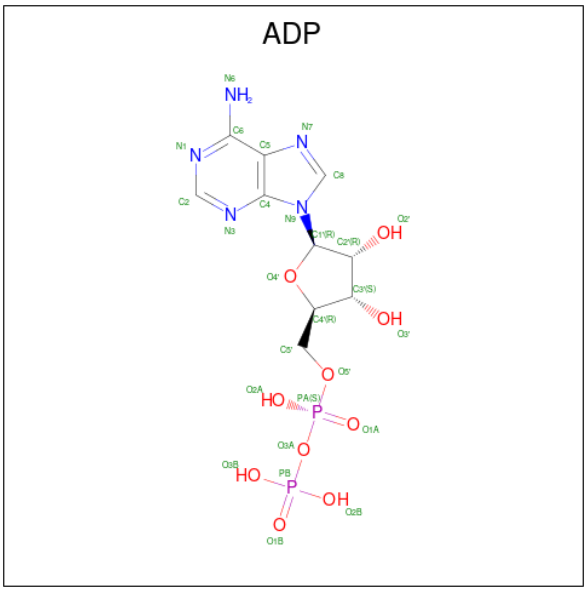
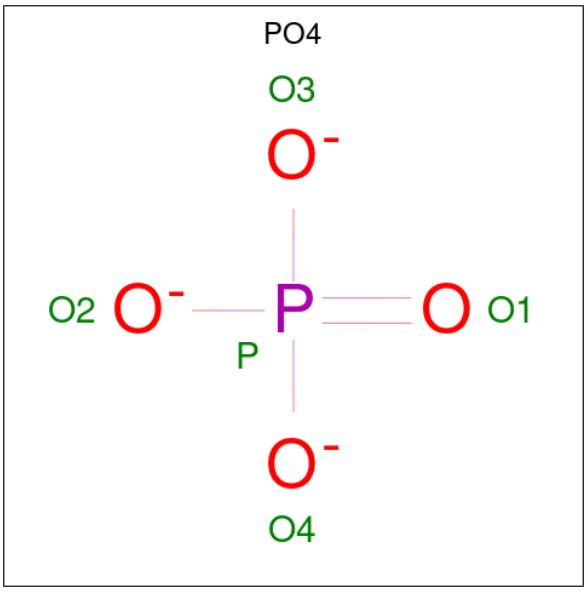
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	C	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
6	F	1	31	10	5	13	3	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	D	1	27	10	5	10	2	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total O P 5 4 1	0	0

- Molecule 9 is water.

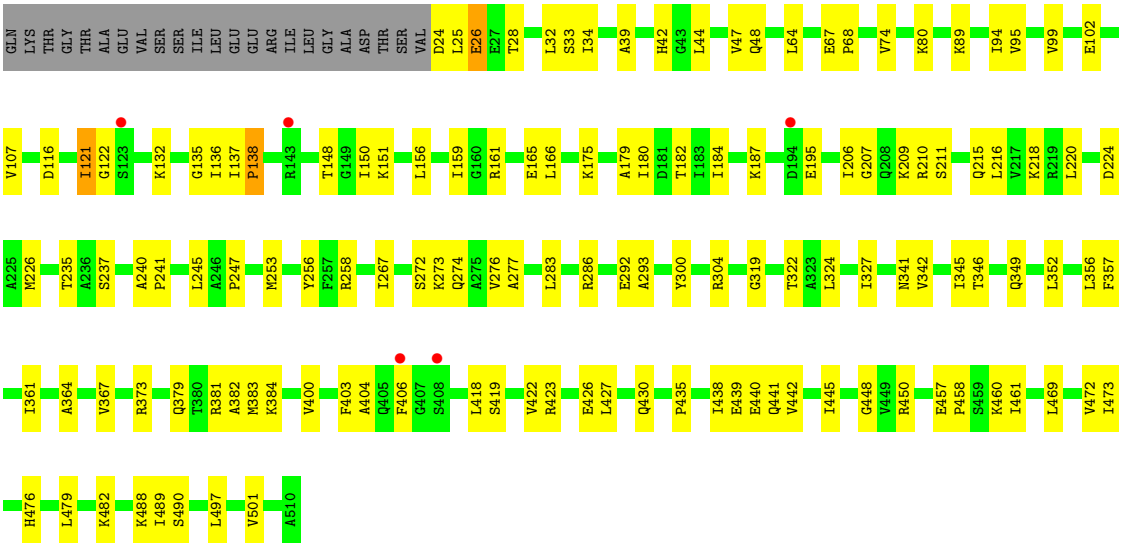
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	35	Total O 35 35	0	0
9	B	34	Total O 34 34	0	0
9	C	28	Total O 28 28	0	0
9	D	19	Total O 19 19	0	0
9	E	21	Total O 21 21	0	0
9	F	26	Total O 26 26	0	0
9	G	1	Total O 1 1	0	0

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.

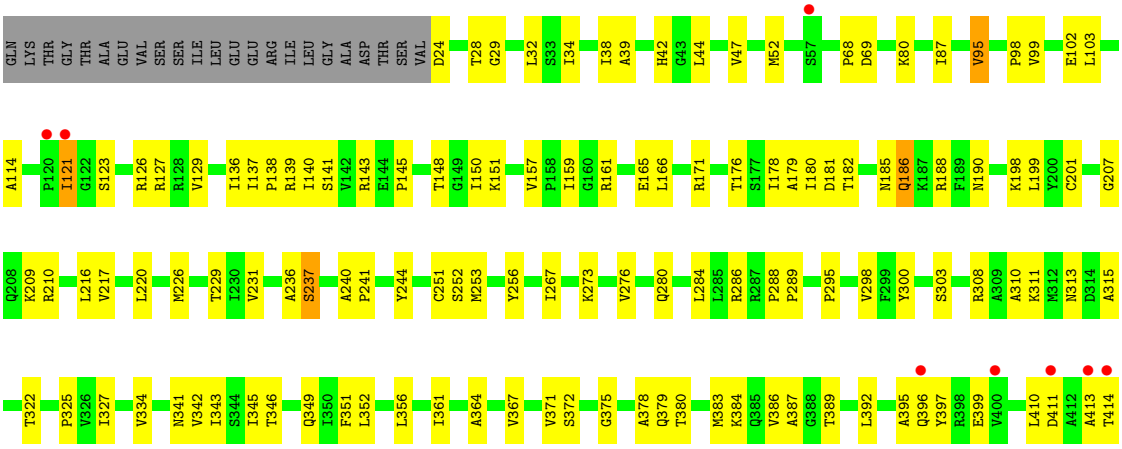
- Molecule 1: F1-ATPASE

Chain A:



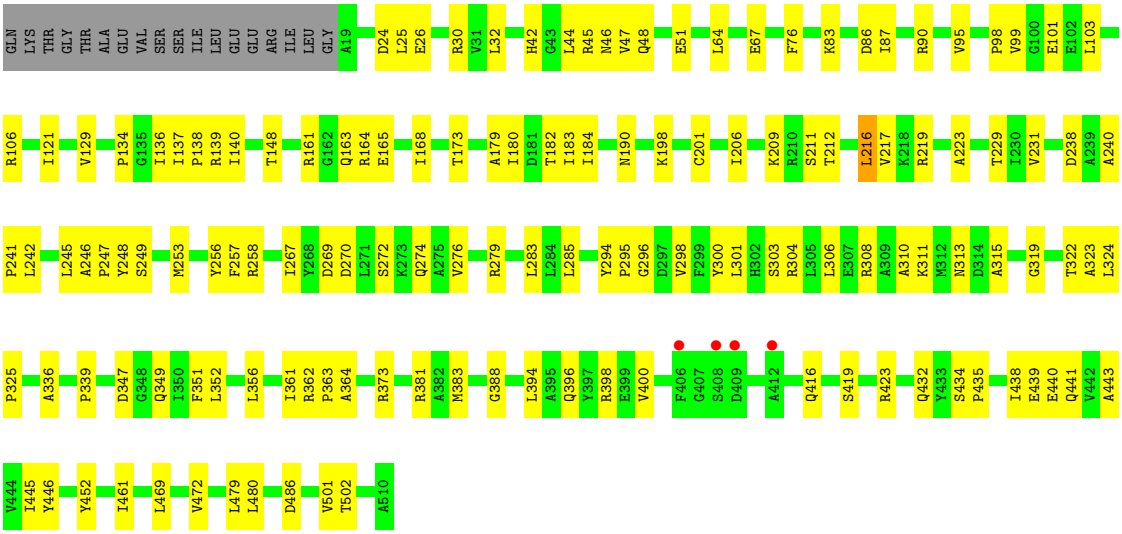
- Molecule 1: F1-ATPASE

Chain B:



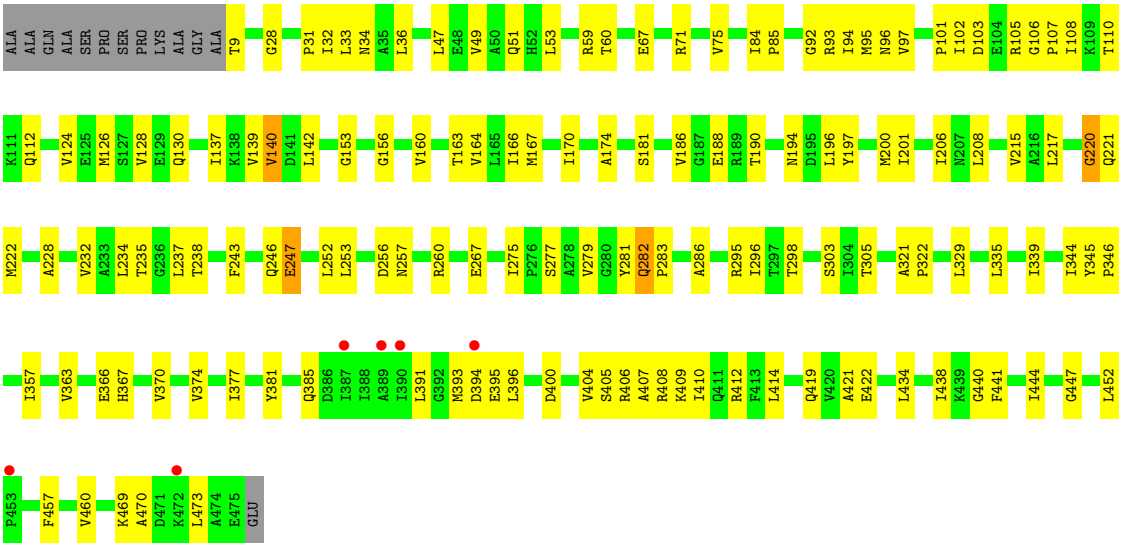
- Molecule 1: F1-ATPASE

Chain C:



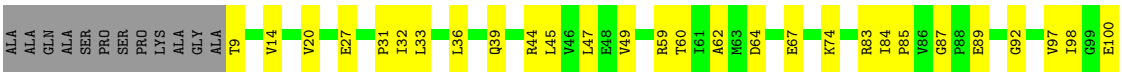
- Molecule 2: F1-ATPASE

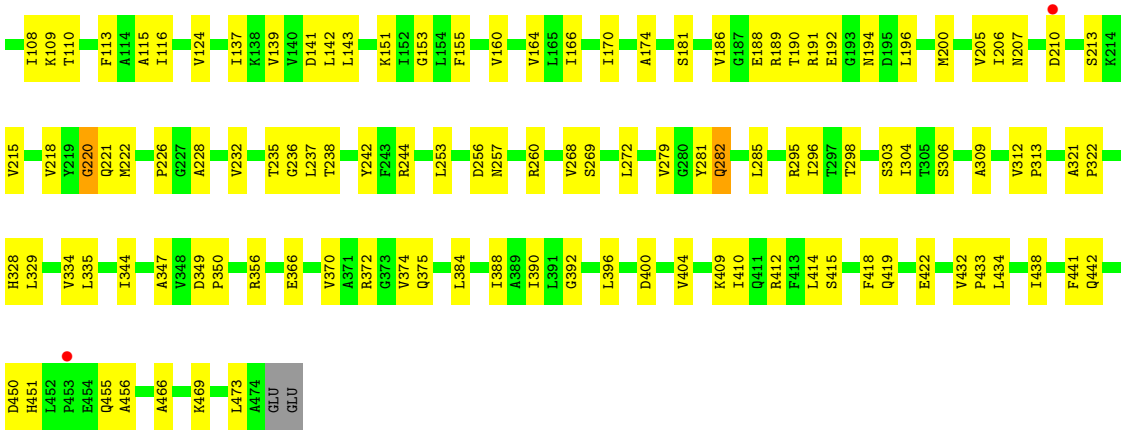
Chain D:



- Molecule 2: F1-ATPASE

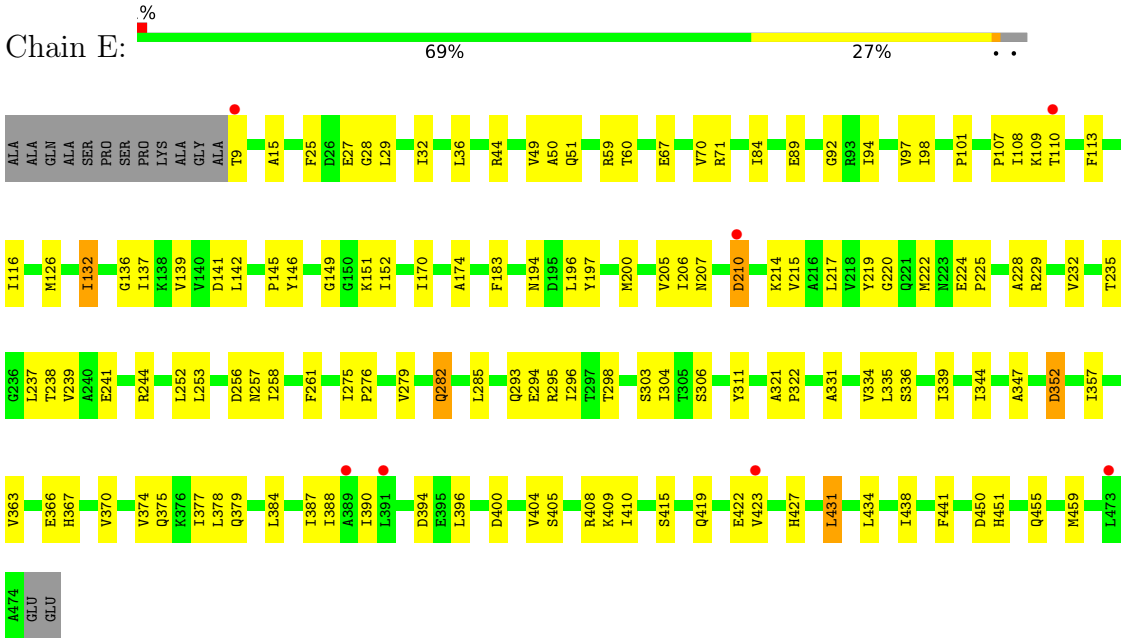
Chain F:





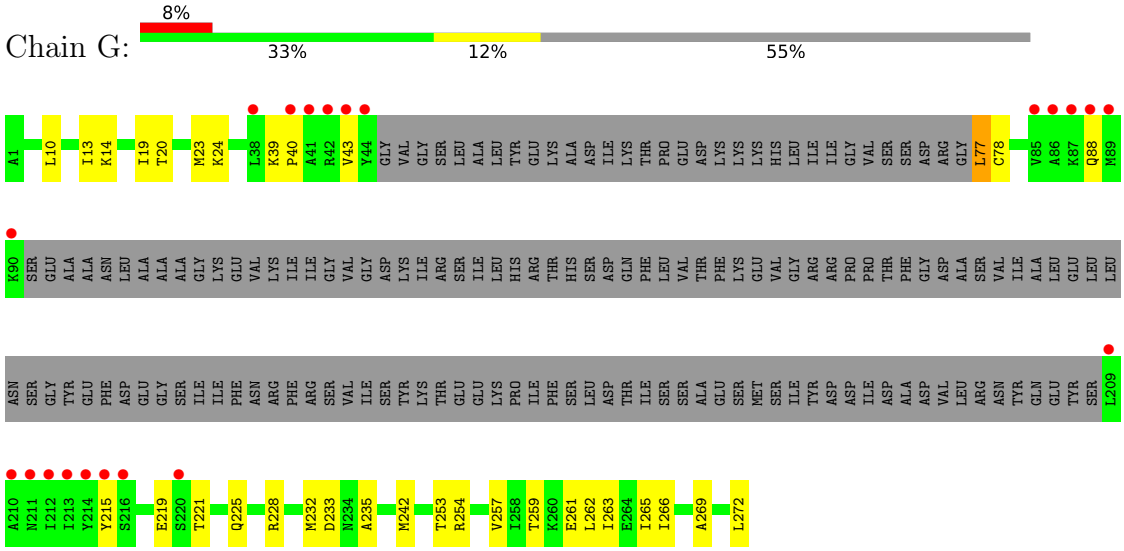
- Molecule 3: F1-ATPASE

Chain E:



- Molecule 4: F1-ATPASE

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	281.00Å 106.60Å 138.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00 29.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.0 (6.00-3.00) 96.6 (29.87-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.207 , 0.297 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 89.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	23057	wwPDB-VP
Average B, all atoms (Å^2)	56.0	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.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TYN, PO4, ADP, 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	0.27	0/3766	0.51	0/5080
1	B	0.27	0/3766	0.51	0/5080
1	C	0.28	0/3799	0.52	0/5126
2	D	0.27	0/3596	0.52	0/4879
2	F	0.27	0/3587	0.53	0/4867
3	E	0.28	0/3573	0.52	0/4846
4	G	0.27	0/949	0.43	0/1266
All	All	0.27	0/23036	0.52	0/31144

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	3715	0	3814	99	0
1	B	3715	0	3814	107	0
1	C	3748	0	3844	99	0
2	D	3539	0	3592	92	0
2	F	3530	0	3586	94	0
3	E	3540	0	3591	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	945	0	1019	21	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	31	0	12	2	0
6	B	31	0	12	1	0
6	C	31	0	12	2	0
6	F	31	0	12	1	0
7	D	27	0	12	1	0
8	E	5	0	0	0	0
9	A	35	0	0	4	0
9	B	34	0	0	1	0
9	C	28	0	0	0	0
9	D	19	0	0	0	0
9	E	21	0	0	2	0
9	F	26	0	0	1	0
9	G	1	0	0	0	0
All	All	23057	0	23320	575	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 12.

All (575) 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:251:CYS:SG	1:B:308:ARG:HD3	1.98	1.03
2:F:220:GLY:HA3	2:F:232:VAL:HG11	1.45	0.97
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.55	0.89
1:B:303:SER:HB2	2:F:222:MET:HB3	1.54	0.87
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.61	0.82
4:G:39:LYS:HB2	4:G:40:PRO:HD3	1.62	0.81
3:E:25:PHE:HB2	3:E:29:LEU:HD12	1.61	0.81
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.62	0.81
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.61	0.81
2:D:49:VAL:HA	2:D:60:THR:HG22	1.63	0.80
3:E:275:ILE:HG23	4:G:266:ILE:HD13	1.63	0.80
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.64	0.79
2:F:388:ILE:HD11	2:F:396:LEU:HD11	1.63	0.78
3:E:170:ILE:HG21	3:E:215:VAL:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:SER:HB2	3:E:294:GLU:HG3	1.65	0.77
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.68	0.74
1:A:357:PHE:HZ	6:A:600:ATP:H1'	1.52	0.73
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.71	0.70
1:B:419:SER:O	1:B:423:ARG:HG2	1.90	0.70
1:A:44:LEU:O	1:A:47:VAL:HG22	1.92	0.70
1:B:352:LEU:HA	1:B:364:ALA:O	1.91	0.70
1:C:432:GLN:OE1	6:C:600:ATP:H2'	1.91	0.70
2:F:298:THR:HG23	2:F:303:SER:HA	1.72	0.69
3:E:97:VAL:HG22	3:E:232:VAL:HG12	1.74	0.69
3:E:101:PRO:HG2	3:E:107:PRO:HA	1.73	0.69
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.75	0.69
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.76	0.68
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.75	0.68
3:E:220:GLY:HA3	3:E:232:VAL:HG11	1.74	0.67
1:B:220:LEU:HB2	1:B:226:MET:HG2	1.76	0.67
2:D:298:THR:HG23	2:D:303:SER:HA	1.75	0.67
1:A:441:GLN:O	1:A:445:ILE:HG12	1.95	0.67
3:E:220:GLY:CA	3:E:232:VAL:HG11	2.24	0.67
2:F:226:PRO:HB2	2:F:268:VAL:HG13	1.77	0.66
1:B:102:GLU:HG3	1:B:123:SER:HA	1.76	0.66
1:B:114:ALA:H	1:B:121:ILE:HD11	1.59	0.66
2:F:196:LEU:O	2:F:200:MET:HG2	1.96	0.66
2:D:101:PRO:HG2	2:D:107:PRO:HA	1.76	0.66
1:A:121:ILE:HD13	1:A:121:ILE:H	1.60	0.66
1:B:32:LEU:HG	1:B:42:HIS:HB2	1.78	0.65
1:C:209:LYS:HE3	1:C:211:SER:HB2	1.79	0.65
1:C:419:SER:O	1:C:423:ARG:HG2	1.96	0.65
1:B:479:LEU:HD23	1:B:496:LYS:HD3	1.79	0.64
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.79	0.64
3:E:84:ILE:HG21	3:E:235:THR:HG23	1.79	0.64
1:B:136:ILE:HG23	2:F:194:ASN:HA	1.79	0.64
2:F:164:VAL:HG23	6:F:600:ATP:O1A	1.97	0.64
2:D:101:PRO:HG3	2:D:108:ILE:HG13	1.81	0.63
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.80	0.63
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.80	0.63
1:B:44:LEU:O	1:B:47:VAL:HG22	1.98	0.63
1:A:381:ARG:HA	1:A:384:LYS:HD2	1.81	0.63
2:F:237:LEU:HD21	2:F:295:ARG:HB2	1.79	0.62
1:C:303:SER:HB2	2:D:222:MET:HB3	1.81	0.62
3:E:422:GLU:HG2	3:E:427:HIS:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:276:PRO:HD2	4:G:266:ILE:HD11	1.80	0.62
1:A:166:LEU:HB2	1:A:346:THR:HG21	1.80	0.62
1:A:150:ILE:HA	1:A:430:GLN:OE1	1.99	0.62
1:B:432:GLN:OE1	6:B:600:ATP:H2'	1.99	0.62
1:A:383:MET:HB2	1:A:438:ILE:HD11	1.81	0.62
1:A:64:LEU:HD12	1:A:74:VAL:HG21	1.82	0.62
3:E:258:ILE:O	3:E:261:PHE:HB3	2.00	0.62
1:C:136:ILE:HG23	2:D:194:ASN:HA	1.82	0.62
1:B:44:LEU:HB3	1:B:47:VAL:CG1	2.29	0.61
1:A:404:ALA:HB2	1:A:418:LEU:HD22	1.80	0.61
1:A:32:LEU:HG	1:A:42:HIS:HB2	1.82	0.61
1:A:206:ILE:HD11	1:A:247:PRO:HD3	1.81	0.61
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.83	0.61
1:B:114:ALA:N	1:B:121:ILE:HD11	2.16	0.61
1:C:44:LEU:O	1:C:47:VAL:HG22	2.01	0.61
3:E:49:VAL:HA	3:E:60:THR:HG22	1.83	0.60
1:C:83:LYS:HD3	2:F:31:PRO:HG3	1.83	0.60
2:F:166:ILE:HD11	2:F:309:ALA:HB2	1.83	0.60
4:G:253:THR:O	4:G:257:VAL:HG23	2.02	0.60
1:B:468:PHE:CZ	1:B:501:VAL:HG12	2.37	0.59
2:D:166:ILE:O	2:D:170:ILE:HG13	2.02	0.59
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.84	0.59
3:E:108:ILE:HG22	3:E:110:THR:HG23	1.85	0.59
2:D:130:GLN:HB3	2:D:357:ILE:HG22	1.84	0.59
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.83	0.59
1:A:211:SER:O	1:A:215:GLN:HG2	2.03	0.59
1:B:343:ILE:HG23	1:B:349:GLN:NE2	2.18	0.59
3:E:151:LYS:HE3	3:E:296:ILE:HB	1.84	0.59
1:B:356:LEU:HB2	1:B:364:ALA:HB1	1.84	0.59
1:B:137:ILE:HB	1:B:138:PRO:HD3	1.85	0.58
3:E:237:LEU:HD21	3:E:295:ARG:HB2	1.84	0.58
1:B:161:ARG:HH12	1:B:199:LEU:HB2	1.69	0.58
1:A:357:PHE:CZ	6:A:600:ATP:H1'	2.36	0.58
1:C:44:LEU:HB3	1:C:47:VAL:HG13	1.85	0.58
3:E:244:ARG:HD3	3:E:304:ILE:HG13	1.85	0.58
1:A:210:ARG:CG	1:A:235:THR:HG21	2.34	0.58
1:A:277:ALA:HB3	9:A:617:HOH:O	2.04	0.58
1:C:296:GLY:O	2:D:267:GLU:HG2	2.04	0.58
1:B:273:LYS:O	1:B:276:VAL:HG22	2.04	0.58
2:D:391:LEU:HD13	4:G:19:ILE:HG21	1.86	0.58
3:E:384:LEU:O	3:E:388:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:384:LEU:O	2:F:388:ILE:HG12	2.04	0.58
1:A:80:LYS:HE2	2:D:33:LEU:HD12	1.86	0.57
1:C:381:ARG:H	1:C:381:ARG:HD2	1.69	0.57
3:E:116:ILE:HA	3:E:238:THR:OG1	2.04	0.57
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.84	0.57
1:C:246:ALA:HB3	1:C:247:PRO:HD3	1.85	0.57
2:D:186:VAL:HG12	2:D:260:ARG:HB2	1.87	0.57
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.86	0.57
1:A:28:THR:HG22	1:A:89:LYS:HG2	1.85	0.57
1:C:98:PRO:O	1:C:103:LEU:HD11	2.05	0.57
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.85	0.57
1:B:80:LYS:HA	3:E:32:ILE:HD12	1.87	0.57
1:C:161:ARG:HA	1:C:322:THR:OG1	2.04	0.57
4:G:215:TYR:O	4:G:219:GLU:HG2	2.04	0.57
2:F:206:ILE:HD11	2:F:215:VAL:HB	1.87	0.56
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.35	0.56
1:C:356:LEU:HB3	1:C:361:ILE:HB	1.87	0.56
2:D:9:THR:HG21	2:D:28:GLY:HA3	1.88	0.56
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.87	0.56
2:D:404:VAL:O	2:D:408:ARG:HG3	2.04	0.56
2:D:469:LYS:O	2:D:473:LEU:HG	2.06	0.56
1:A:379:GLN:O	1:A:384:LYS:HE3	2.05	0.56
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.87	0.56
3:E:183:PHE:HB3	3:E:217:LEU:HD23	1.87	0.56
1:A:210:ARG:HG3	1:A:235:THR:HG21	1.87	0.56
3:E:387:ILE:H	3:E:387:ILE:HD12	1.71	0.55
1:B:151:LYS:HE2	1:B:436:MET:SD	2.47	0.55
1:C:26:GLU:O	1:C:46:ASN:HB2	2.06	0.55
2:F:419:GLN:HA	2:F:422:GLU:HG3	1.87	0.55
1:A:422:VAL:HG23	1:A:423:ARG:HD2	1.87	0.55
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.41	0.55
1:C:99:VAL:HG11	1:C:256:TYR:HB2	1.89	0.55
3:E:36:LEU:HD12	3:E:60:THR:HG21	1.87	0.55
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.87	0.55
2:D:188:GLU:O	2:D:221:GLN:HB3	2.07	0.55
1:B:300:TYR:HA	1:B:303:SER:OG	2.07	0.54
2:F:282:GLN:H	2:F:282:GLN:NE2	2.05	0.54
1:B:441:GLN:O	1:B:445:ILE:HG12	2.07	0.54
2:D:282:GLN:H	2:D:282:GLN:NE2	2.06	0.54
3:E:141:ASP:HB3	3:E:434:LEU:HD13	1.89	0.54
1:A:195:GLU:HG3	9:A:609:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ARG:O	1:C:319:GLY:HA3	2.07	0.54
2:D:234:LEU:HD22	2:D:295:ARG:NH1	2.22	0.54
1:C:134:PRO:HG3	1:C:258:ARG:HH12	1.71	0.54
2:F:108:ILE:HG22	2:F:110:THR:HG23	1.89	0.54
2:F:116:ILE:HA	2:F:238:THR:OG1	2.08	0.54
2:D:253:LEU:HD23	2:D:296:ILE:HG23	1.89	0.54
4:G:20:THR:HG21	4:G:235:ALA:HB3	1.89	0.54
3:E:228:ALA:O	3:E:232:VAL:HG13	2.08	0.54
1:C:64:LEU:HD23	1:C:285:LEU:HD11	1.90	0.54
2:D:396:LEU:HB3	2:D:400:ASP:HB2	1.89	0.54
1:A:419:SER:O	1:A:423:ARG:HD3	2.07	0.54
2:D:252:LEU:HD23	2:D:305:THR:HB	1.90	0.54
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.73	0.53
3:E:101:PRO:HG3	3:E:108:ILE:HG13	1.89	0.53
1:A:300:TYR:HB2	9:E:604:HOH:O	2.08	0.53
3:E:377:ILE:HG21	3:E:410:ILE:HD12	1.90	0.53
2:F:285:LEU:HB3	9:F:624:HOH:O	2.08	0.53
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.90	0.53
2:F:190:THR:HA	2:F:221:GLN:HG3	1.90	0.53
1:A:422:VAL:O	1:A:426:GLU:HG2	2.08	0.53
1:C:164:ARG:HD2	1:C:306:LEU:HB3	1.90	0.53
2:D:139:VAL:HG22	2:D:414:LEU:HB3	1.90	0.53
1:A:215:GLN:HE22	2:D:128:VAL:HA	1.73	0.53
1:A:258:ARG:O	1:A:319:GLY:HA3	2.08	0.53
2:D:366:GLU:O	2:D:370:VAL:HG23	2.09	0.53
2:F:49:VAL:HA	2:F:60:THR:HG22	1.90	0.53
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.44	0.53
2:D:167:MET:SD	2:D:196:LEU:HD13	2.48	0.53
2:D:190:THR:HA	2:D:221:GLN:HG3	1.91	0.53
1:B:497:LEU:HA	1:B:500:ILE:HD12	1.90	0.53
1:A:240:ALA:N	1:A:241:PRO:HD2	2.24	0.53
2:D:163:THR:O	2:D:166:ILE:HG22	2.09	0.53
1:C:44:LEU:HB3	1:C:47:VAL:CG1	2.39	0.52
1:C:168:ILE:HG23	1:C:351:PHE:HD1	1.74	0.52
1:C:164:ARG:HA	1:C:323:ALA:O	2.10	0.52
1:C:201:CYS:O	1:C:229:THR:HA	2.09	0.52
3:E:44:ARG:HE	3:E:98:ILE:HD12	1.74	0.52
2:F:400:ASP:O	2:F:404:VAL:HG23	2.10	0.52
2:D:97:VAL:HG21	2:D:228:ALA:HB1	1.92	0.52
1:C:47:VAL:HA	1:C:90:ARG:HE	1.74	0.52
1:B:452:TYR:CE2	1:B:501:VAL:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:PHE:O	2:D:247:GLU:HB3	2.10	0.52
2:F:434:LEU:O	2:F:438:ILE:HG12	2.10	0.52
1:A:341:ASN:O	1:A:345:ILE:HG13	2.10	0.52
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.91	0.52
3:E:282:GLN:H	3:E:282:GLN:NE2	2.08	0.52
2:F:85:PRO:HG3	2:F:113:PHE:HE1	1.75	0.52
9:A:627:HOH:O	2:D:286:ALA:HB3	2.10	0.52
1:B:383:MET:HG2	1:B:438:ILE:HD11	1.91	0.52
1:B:161:ARG:NH1	1:B:199:LEU:HB2	2.24	0.51
1:C:165:GLU:O	1:C:325:PRO:HD2	2.10	0.51
2:D:36:LEU:HB2	2:D:47:LEU:HB2	1.92	0.51
3:E:170:ILE:HG21	3:E:215:VAL:CG2	2.39	0.51
3:E:237:LEU:O	3:E:241:GLU:HG3	2.10	0.51
3:E:253:LEU:O	3:E:306:SER:HA	2.10	0.51
2:D:156:GLY:HA3	2:D:160:VAL:HG21	1.91	0.51
3:E:335:LEU:HA	3:E:347:ALA:O	2.10	0.51
1:C:148:THR:HA	1:C:182:THR:HG23	1.91	0.51
1:C:394:LEU:O	1:C:398:ARG:HG3	2.10	0.51
1:C:434:SER:N	1:C:435:PRO:HD3	2.26	0.51
3:E:142:LEU:HD21	3:E:374:VAL:HG21	1.92	0.51
3:E:207:ASN:HB3	3:E:210:ASP:O	2.10	0.51
3:E:282:GLN:NE2	3:E:285:LEU:HD13	2.26	0.51
2:F:390:ILE:HD11	4:G:242:MET:SD	2.51	0.51
1:A:300:TYR:O	1:A:304:ARG:HG2	2.11	0.51
1:C:165:GLU:HB3	1:C:324:LEU:HD22	1.93	0.51
1:C:432:GLN:HG3	6:C:600:ATP:C5	2.46	0.51
3:E:136:GLY:HA3	3:E:431:LEU:HD13	1.93	0.50
1:B:447:ALA:HA	1:B:452:TYR:HD2	1.76	0.50
1:C:373:ARG:HA	7:D:600:ADP:O3'	2.11	0.50
2:D:452:LEU:HD22	2:D:470:ALA:CB	2.41	0.50
3:E:276:PRO:HB2	4:G:262:LEU:HD21	1.93	0.50
1:A:215:GLN:NE2	2:D:128:VAL:HA	2.26	0.50
1:B:343:ILE:HG23	1:B:349:GLN:HE21	1.75	0.50
1:C:248:TYR:OH	1:C:301:LEU:HD12	2.12	0.50
2:F:388:ILE:HA	2:F:392:GLY:O	2.11	0.50
1:A:210:ARG:HB2	2:D:126:MET:HE2	1.93	0.50
2:F:97:VAL:HG23	2:F:98:ILE:HG23	1.93	0.50
1:C:164:ARG:HD3	1:C:306:LEU:O	2.12	0.50
2:F:366:GLU:O	2:F:370:VAL:HG23	2.11	0.50
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.94	0.49
2:F:191:ARG:HG3	2:F:192:GLU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PRO:HA	1:A:461:ILE:HG12	1.94	0.49
3:E:84:ILE:HD13	3:E:235:THR:HG23	1.93	0.49
1:B:99:VAL:HG21	1:B:127:ARG:CB	2.41	0.49
1:B:295:PRO:HG2	1:B:298:VAL:HG13	1.95	0.49
3:E:97:VAL:HG22	3:E:232:VAL:CG1	2.42	0.49
1:C:206:ILE:HG21	1:C:274:GLN:HB2	1.94	0.49
1:C:217:VAL:HG12	1:C:231:VAL:HG21	1.94	0.49
3:E:404:VAL:O	3:E:408:ARG:HG3	2.13	0.49
2:F:142:LEU:HD22	2:F:441:PHE:CD2	2.46	0.49
1:A:180:ILE:O	1:A:184:ILE:HG12	2.13	0.49
1:B:397:TYR:HD1	1:B:418:LEU:HA	1.76	0.49
1:C:140:ILE:HG22	1:C:311:LYS:HG3	1.95	0.49
4:G:77:LEU:HD23	4:G:77:LEU:N	2.28	0.49
1:A:94:ILE:HG12	1:A:95:VAL:H	1.77	0.49
1:A:403:PHE:N	1:A:403:PHE:CD1	2.80	0.49
1:C:383:MET:HB2	1:C:438:ILE:HD11	1.95	0.49
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.95	0.49
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.93	0.49
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.93	0.49
2:F:253:LEU:HD23	2:F:296:ILE:HG23	1.94	0.49
1:B:356:LEU:HB3	1:B:361:ILE:HB	1.95	0.49
1:C:441:GLN:O	1:C:445:ILE:HG12	2.12	0.49
2:F:9:THR:N	2:F:27:GLU:O	2.45	0.49
1:A:34:ILE:HD13	1:A:39:ALA:HB2	1.95	0.48
1:B:34:ILE:HD13	1:B:39:ALA:HB2	1.95	0.48
1:B:103:LEU:HD23	1:B:253:MET:SD	2.53	0.48
1:C:99:VAL:HG13	1:C:253:MET:HA	1.94	0.48
2:D:153:GLY:HA3	2:D:329:LEU:HD13	1.95	0.48
3:E:32:ILE:HG23	3:E:50:ALA:HA	1.95	0.48
1:A:427:LEU:HD11	1:A:448:GLY:HA3	1.96	0.48
2:D:370:VAL:HG21	2:D:438:ILE:HG23	1.94	0.48
3:E:400:ASP:O	3:E:404:VAL:HG23	2.14	0.48
2:F:188:GLU:O	2:F:221:GLN:HB3	2.13	0.48
2:F:456:ALA:O	2:F:466:ALA:HA	2.13	0.48
1:A:382:ALA:HA	1:A:488:LYS:HA	1.95	0.48
1:B:207:GLY:O	1:B:236:ALA:HB2	2.12	0.48
1:B:209:LYS:HE3	9:E:618:HOH:O	2.13	0.48
3:E:9:THR:HG21	3:E:27:GLU:O	2.13	0.48
1:C:298:VAL:O	1:C:301:LEU:HB3	2.13	0.48
1:A:99:VAL:HG21	1:A:256:TYR:HB2	1.94	0.48
2:F:141:ASP:HB3	2:F:434:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.77	0.48
2:D:277:SER:HB3	2:D:281:TYR:O	2.14	0.48
3:E:396:LEU:HB3	3:E:400:ASP:HB2	1.95	0.48
1:A:211:SER:N	2:D:126:MET:HE3	2.29	0.48
1:C:347:ASP:HA	1:C:373:ARG:HD2	1.96	0.48
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.43	0.48
2:F:335:LEU:HA	2:F:347:ALA:O	2.13	0.48
1:B:186:GLN:CG	1:B:199:LEU:HB3	2.43	0.48
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.95	0.48
2:F:36:LEU:HD12	2:F:60:THR:HG21	1.96	0.48
1:B:453:LEU:HB3	1:B:461:ILE:HD12	1.95	0.47
3:E:367:HIS:CE1	3:E:434:LEU:HD11	2.48	0.47
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.96	0.47
1:C:206:ILE:CD1	1:C:247:PRO:HG3	2.43	0.47
2:D:339:ILE:HG22	2:D:344:ILE:HB	1.96	0.47
3:E:132:ILE:HD12	3:E:145:PRO:HB3	1.96	0.47
3:E:339:ILE:HG22	3:E:344:ILE:HB	1.96	0.47
2:F:155:PHE:HB2	2:F:334:VAL:HA	1.95	0.47
1:B:166:LEU:HB2	1:B:346:THR:HG21	1.97	0.47
3:E:229:ARG:O	3:E:232:VAL:HG22	2.15	0.47
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.45	0.47
1:B:145:PRO:HB3	1:B:378:ALA:O	2.14	0.47
1:C:206:ILE:HD11	1:C:247:PRO:HG3	1.97	0.47
2:F:170:ILE:O	2:F:174:ALA:HB3	2.15	0.47
2:F:256:ASP:HA	2:F:257:ASN:HA	1.70	0.47
2:F:412:ARG:HG3	2:F:412:ARG:HH11	1.80	0.47
4:G:221:THR:O	4:G:225:GLN:HG2	2.15	0.47
1:A:403:PHE:N	1:A:403:PHE:HD1	2.12	0.47
1:B:201:CYS:O	1:B:229:THR:HA	2.15	0.47
1:B:327:ILE:HD11	1:B:342:VAL:HG21	1.96	0.47
2:D:160:VAL:HB	2:D:335:LEU:HB3	1.96	0.47
2:F:281:TYR:HD1	2:F:282:GLN:HE22	1.63	0.47
1:B:150:ILE:HD12	1:B:178:ILE:HG23	1.96	0.47
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.97	0.47
2:F:39:GLN:HB2	2:F:74:LYS:HB2	1.97	0.47
2:F:200:MET:HB3	2:F:206:ILE:HG12	1.96	0.47
2:F:205:VAL:O	2:F:213:SER:HA	2.15	0.47
2:F:253:LEU:O	2:F:306:SER:HA	2.15	0.47
1:B:453:LEU:HD13	1:B:461:ILE:HG23	1.96	0.47
2:F:32:ILE:O	2:F:33:LEU:HB2	2.15	0.47
3:E:149:GLY:HA3	3:E:298:THR:OG1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:170:ILE:HD13	3:E:215:VAL:CG2	2.45	0.46
3:E:298:THR:HG23	3:E:303:SER:HB3	1.96	0.46
3:E:374:VAL:HG13	3:E:410:ILE:HG21	1.98	0.46
1:B:165:GLU:O	1:B:325:PRO:HD2	2.15	0.46
1:B:176:THR:HG21	9:B:631:HOH:O	2.15	0.46
2:F:189:ARG:HB2	2:F:192:GLU:HG3	1.97	0.46
1:A:99:VAL:CG2	1:A:253:MET:HA	2.45	0.46
2:D:377:ILE:HG12	2:D:407:ALA:HB2	1.97	0.46
3:E:419:GLN:HA	3:E:422:GLU:HG3	1.97	0.46
1:A:352:LEU:HA	1:A:364:ALA:O	2.15	0.46
1:B:371:VAL:HG12	1:B:372:SER:N	2.31	0.46
1:C:32:LEU:HG	1:C:42:HIS:HB2	1.98	0.46
3:E:152:ILE:HG13	3:E:331:ALA:HB3	1.97	0.46
2:F:87:GLY:HA2	2:F:242:TYR:CE1	2.50	0.46
1:B:32:LEU:CG	1:B:42:HIS:HB2	2.46	0.46
3:E:116:ILE:HG22	3:E:235:THR:HA	1.97	0.46
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.98	0.46
1:C:184:ILE:HG23	1:C:223:ALA:HB1	1.98	0.46
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.98	0.46
2:D:256:ASP:HA	2:D:257:ASN:HA	1.67	0.46
2:D:440:GLY:O	2:D:444:ILE:HG13	2.14	0.46
1:B:468:PHE:O	1:B:471:HIS:HB3	2.15	0.46
2:F:200:MET:CE	2:F:215:VAL:HG11	2.46	0.46
1:B:185:ASN:HB2	1:B:435:PRO:HB3	1.97	0.46
1:B:469:LEU:O	1:B:473:ILE:HG13	2.15	0.46
3:E:94:ILE:HD11	3:E:197:TYR:CG	2.51	0.46
3:E:256:ASP:HA	3:E:257:ASN:HA	1.52	0.46
4:G:23:MET:SD	4:G:232:MET:HE1	2.56	0.46
1:A:272:SER:O	1:A:276:VAL:HG23	2.15	0.46
1:A:349:GLN:HE22	1:A:373:ARG:HH12	1.64	0.46
1:A:48:GLN:HG2	3:E:70:VAL:HG22	1.98	0.46
2:D:92:GLY:HA2	2:D:206:ILE:HG23	1.98	0.46
2:F:269:SER:HA	2:F:272:LEU:HD12	1.97	0.46
1:A:48:GLN:HG2	3:E:70:VAL:CG2	2.45	0.45
1:A:220:LEU:CB	1:A:226:MET:HG2	2.45	0.45
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.98	0.45
1:B:139:ARG:NH1	1:B:310:ALA:HB2	2.31	0.45
1:B:288:PRO:HA	1:B:289:PRO:HD2	1.88	0.45
1:B:334:VAL:HG11	1:B:351:PHE:CE2	2.52	0.45
1:C:47:VAL:HG12	1:C:90:ARG:HG2	1.96	0.45
1:C:95:VAL:O	1:C:129:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:GLU:HB3	1:C:469:LEU:HD11	1.99	0.45
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.46	0.45
1:B:159:ILE:HD12	1:B:165:GLU:HG2	1.98	0.45
1:C:140:ILE:CG2	1:C:311:LYS:HG3	2.46	0.45
1:C:362:ARG:HA	1:C:363:PRO:C	2.35	0.45
2:D:164:VAL:HG11	2:D:421:ALA:HB2	1.97	0.45
3:E:375:GLN:O	3:E:379:GLN:HG3	2.17	0.45
4:G:39:LYS:O	4:G:43:VAL:HG23	2.15	0.45
1:A:286:ARG:HH12	4:G:272:LEU:HD13	1.81	0.45
1:B:286:ARG:HA	3:E:275:ILE:HD12	1.98	0.45
1:C:95:VAL:HG11	1:C:245:LEU:HD21	1.99	0.45
2:D:103:ASP:OD2	2:D:105:ARG:HB2	2.17	0.45
3:E:89:GLU:HG3	3:E:109:LYS:O	2.16	0.45
1:B:44:LEU:HB3	1:B:47:VAL:HG11	1.98	0.45
3:E:92:GLY:HA2	3:E:206:ILE:HG23	1.97	0.45
3:E:145:PRO:HB2	3:E:357:ILE:HD11	1.99	0.45
2:F:200:MET:HE3	2:F:215:VAL:HG11	1.99	0.45
2:D:94:ILE:HB	2:D:103:ASP:HB3	1.99	0.45
2:D:381:TYR:O	2:D:385:GLN:HG3	2.15	0.45
1:B:386:VAL:HG23	1:B:387:ALA:N	2.32	0.45
2:D:85:PRO:HG2	2:D:95:MET:SD	2.57	0.45
1:C:267:ILE:N	1:C:267:ILE:HD12	2.32	0.45
3:E:374:VAL:O	3:E:377:ILE:HG22	2.17	0.45
2:F:84:ILE:HD11	2:F:238:THR:HB	1.98	0.45
2:F:89:GLU:HB2	2:F:110:THR:HG22	1.99	0.45
2:F:438:ILE:O	2:F:442:GLN:HG3	2.17	0.45
1:B:24:ASP:O	1:B:28:THR:HB	2.18	0.45
1:B:68:PRO:HG3	2:F:14:VAL:O	2.17	0.45
3:E:224:GLU:O	3:E:229:ARG:NH1	2.49	0.45
1:C:48:GLN:HB2	1:C:51:GLU:HB2	1.99	0.44
1:C:362:ARG:NH2	2:F:372:ARG:HD2	2.31	0.44
1:C:443:ALA:O	1:C:446:TYR:HB3	2.17	0.44
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.52	0.44
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.99	0.44
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.99	0.44
1:C:173:THR:HB	1:C:352:LEU:HB2	2.00	0.44
1:C:398:ARG:HG2	1:C:398:ARG:HH11	1.81	0.44
2:D:396:LEU:HB3	2:D:400:ASP:CB	2.48	0.44
2:D:419:GLN:HA	2:D:422:GLU:HG3	1.98	0.44
3:E:415:SER:HB2	3:E:459:MET:SD	2.58	0.44
1:A:32:LEU:CG	1:A:42:HIS:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ASP:HB3	1:C:242:LEU:HD12	1.99	0.44
2:D:197:TYR:O	2:D:201:ILE:HG13	2.17	0.44
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.99	0.44
2:F:412:ARG:HG3	2:F:412:ARG:NH1	2.33	0.44
1:A:68:PRO:HD3	3:E:15:ALA:HB2	1.99	0.44
1:A:283:LEU:HD12	2:D:283:PRO:HB3	2.00	0.44
1:B:472:VAL:O	1:B:476:HIS:HB2	2.17	0.44
1:A:148:THR:HA	1:A:182:THR:HG23	2.00	0.44
1:B:395:ALA:O	1:B:399:GLU:HG3	2.15	0.44
3:E:196:LEU:O	3:E:200:MET:HG3	2.17	0.44
2:F:432:VAL:HA	2:F:433:PRO:HD3	1.87	0.44
4:G:261:GLU:O	4:G:265:ILE:HG13	2.18	0.44
1:B:157:VAL:HG13	1:B:372:SER:HB2	2.00	0.44
1:C:272:SER:O	1:C:276:VAL:HG23	2.17	0.44
1:C:439:GLU:HG3	1:C:480:LEU:HB3	1.99	0.44
3:E:334:VAL:HG21	3:E:352:ASP:HB3	2.00	0.44
3:E:366:GLU:O	3:E:370:VAL:HG23	2.18	0.44
1:A:99:VAL:HG23	1:A:253:MET:HA	1.99	0.44
2:D:367:HIS:CE1	2:D:434:LEU:HD11	2.53	0.44
2:F:189:ARG:HA	2:F:222:MET:HE2	1.98	0.44
1:A:33:SER:HB3	2:D:53:LEU:O	2.17	0.44
1:A:137:ILE:HB	1:A:138:PRO:HD3	1.99	0.44
1:A:472:VAL:HA	1:A:476:HIS:HB2	2.00	0.44
1:B:140:ILE:CG2	1:B:311:LYS:HG3	2.47	0.44
1:C:168:ILE:HG23	1:C:351:PHE:CD1	2.52	0.44
1:C:183:ILE:HD11	1:C:267:ILE:HD13	2.00	0.44
1:C:279:ARG:O	1:C:283:LEU:HG	2.18	0.44
1:C:336:ALA:HB3	1:C:339:PRO:HD2	1.99	0.44
3:E:132:ILE:CD1	3:E:145:PRO:HB3	2.47	0.44
3:E:336:SER:HB3	3:E:339:ILE:HG12	1.99	0.43
2:F:143:LEU:HD22	2:F:375:GLN:HG3	2.00	0.43
2:F:97:VAL:HG11	2:F:228:ALA:HA	2.00	0.43
2:D:237:LEU:HD21	2:D:295:ARG:HB2	2.01	0.43
2:F:160:VAL:HG11	2:F:335:LEU:HB3	1.99	0.43
1:A:210:ARG:HG2	1:A:235:THR:HG21	2.00	0.43
1:C:300:TYR:HA	1:C:303:SER:OG	2.18	0.43
1:C:304:ARG:O	1:C:308:ARG:HG3	2.19	0.43
2:D:51:GLN:OE1	2:D:59:ARG:HD2	2.18	0.43
2:D:275:ILE:HG23	4:G:269:ALA:HB2	2.00	0.43
3:E:434:LEU:O	3:E:438:ILE:HG12	2.18	0.43
2:F:45:LEU:HD13	2:F:64:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLY:C	1:A:138:PRO:HD2	2.38	0.43
1:A:489:ILE:HD12	1:A:489:ILE:N	2.34	0.43
1:C:32:LEU:CG	1:C:42:HIS:HB2	2.49	0.43
1:C:269:ASP:HA	1:C:270:ASP:HA	1.72	0.43
2:F:47:LEU:HD23	2:F:62:ALA:HA	1.99	0.43
2:F:220:GLY:CA	2:F:232:VAL:HG11	2.33	0.43
2:F:469:LYS:O	2:F:473:LEU:HG	2.18	0.43
1:C:163:GLN:HG2	1:C:164:ARG:N	2.33	0.43
3:E:222:MET:HA	3:E:229:ARG:HD3	2.01	0.43
4:G:13:ILE:HD13	4:G:242:MET:SD	2.59	0.43
1:A:161:ARG:HA	1:A:322:THR:OG1	2.19	0.43
1:B:140:ILE:HG13	1:B:141:SER:N	2.33	0.43
1:C:45:ARG:HH21	2:D:71:ARG:NE	2.16	0.43
1:C:76:PHE:HE2	1:C:245:LEU:HD22	1.83	0.43
3:E:170:ILE:HD13	3:E:215:VAL:HG22	2.01	0.43
3:E:196:LEU:HD23	3:E:219:TYR:OH	2.18	0.43
2:F:36:LEU:HB2	2:F:47:LEU:HB2	1.99	0.43
1:A:469:LEU:O	1:A:473:ILE:HG13	2.19	0.43
2:D:137:ILE:HB	2:D:140:VAL:HB	2.00	0.43
1:B:396:GLN:HB3	1:B:417:LEU:HD13	2.01	0.43
2:F:207:ASN:HB3	2:F:210:ASP:O	2.19	0.43
2:F:409:LYS:NZ	2:F:450:ASP:HA	2.34	0.43
1:A:67:GLU:O	3:E:71:ARG:NH1	2.51	0.43
1:A:107:VAL:HB	1:A:116:ASP:HB3	2.01	0.43
1:B:280:GLN:O	1:B:284:LEU:HG	2.19	0.43
2:D:181:SER:HB2	2:D:215:VAL:HG22	2.00	0.43
2:D:96:ASN:HB2	2:D:102:ILE:HG23	2.01	0.42
1:A:102:GLU:HG3	1:A:122:GLY:O	2.19	0.42
1:A:209:LYS:HE3	1:A:211:SER:HB2	2.02	0.42
1:A:430:GLN:NE2	1:A:435:PRO:HA	2.34	0.42
1:C:30:ARG:HA	1:C:86:ASP:O	2.19	0.42
1:C:352:LEU:HA	1:C:364:ALA:O	2.19	0.42
2:D:31:PRO:O	2:D:34:ASN:HB2	2.19	0.42
2:D:84:ILE:HD11	2:D:238:THR:HB	2.00	0.42
2:F:207:ASN:ND2	2:F:210:ASP:HB2	2.34	0.42
1:B:28:THR:HG22	1:B:29:GLY:N	2.34	0.42
1:B:148:THR:HA	1:B:182:THR:HG23	2.01	0.42
2:D:357:ILE:O	2:D:363:VAL:HG13	2.19	0.42
1:A:175:LYS:HB2	1:A:175:LYS:HE3	1.89	0.42
1:A:187:LYS:NZ	1:A:224:ASP:HB3	2.35	0.42
1:B:313:ASN:OD1	1:B:315:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:GLN:O	2:D:247:GLU:HB2	2.20	0.42
2:D:344:ILE:HD12	2:D:412:ARG:HA	2.00	0.42
3:E:151:LYS:HD2	3:E:151:LYS:N	2.35	0.42
3:E:174:ALA:HB3	3:E:214:LYS:HD3	1.99	0.42
3:E:205:VAL:HG23	3:E:206:ILE:HG13	2.01	0.42
2:F:139:VAL:HG22	2:F:414:LEU:HB3	2.01	0.42
2:F:186:VAL:HG12	2:F:260:ARG:HB2	2.00	0.42
1:A:95:VAL:HG11	1:A:245:LEU:HD13	2.02	0.42
1:A:165:GLU:O	1:A:324:LEU:HA	2.20	0.42
1:A:497:LEU:O	1:A:501:VAL:HG22	2.19	0.42
1:C:165:GLU:HB3	1:C:324:LEU:CD2	2.49	0.42
2:D:345:TYR:HA	2:D:346:PRO:C	2.40	0.42
3:E:387:ILE:HD12	3:E:387:ILE:N	2.35	0.42
1:C:212:THR:HA	2:F:356:ARG:HH22	1.83	0.42
2:D:94:ILE:HG12	2:D:217:LEU:HD12	2.01	0.42
2:D:108:ILE:HG22	2:D:110:THR:HG23	2.01	0.42
2:D:457:PHE:O	2:D:460:VAL:HG22	2.20	0.42
1:A:218:LYS:HG3	2:D:128:VAL:HG21	2.02	0.42
1:B:439:GLU:HG2	1:B:440:GLU:N	2.35	0.42
1:C:137:ILE:HB	1:C:138:PRO:HD3	2.01	0.42
3:E:321:ALA:HB3	3:E:322:PRO:CD	2.50	0.42
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.20	0.42
2:F:83:ARG:HA	2:F:115:ALA:HA	2.01	0.42
2:F:89:GLU:HG3	2:F:109:LYS:O	2.19	0.42
1:A:136:ILE:O	3:E:194:ASN:ND2	2.52	0.42
1:B:478:ALA:O	1:B:482:LYS:HG3	2.20	0.42
1:C:24:ASP:C	1:C:26:GLU:H	2.23	0.42
1:C:101:GLU:HG2	1:C:257:PHE:HE1	1.84	0.42
1:C:438:ILE:HG23	1:C:439:GLU:N	2.35	0.42
1:C:168:ILE:O	1:C:351:PHE:HA	2.19	0.41
3:E:146:TYR:CD1	3:E:152:ILE:HG12	2.55	0.41
1:A:450:ARG:HD3	1:A:450:ARG:HA	1.89	0.41
1:B:210:ARG:HB3	3:E:126:MET:HG3	2.02	0.41
2:F:160:VAL:CG1	2:F:335:LEU:HB3	2.50	0.41
2:F:244:ARG:HD3	2:F:304:ILE:CD1	2.49	0.41
1:B:161:ARG:HA	1:B:322:THR:OG1	2.19	0.41
1:C:87:ILE:N	1:C:87:ILE:HD12	2.35	0.41
2:D:36:LEU:HB3	2:D:75:VAL:CG1	2.50	0.41
2:D:170:ILE:O	2:D:174:ALA:HB3	2.21	0.41
3:E:51:GLN:HB3	3:E:59:ARG:HB3	2.02	0.41
3:E:235:THR:O	3:E:239:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:374:VAL:O	3:E:378:LEU:HG	2.20	0.41
4:G:78:CYS:SG	4:G:228:ARG:NH2	2.94	0.41
1:B:129:VAL:HA	1:B:252:SER:OG	2.21	0.41
2:D:370:VAL:O	2:D:374:VAL:HG23	2.20	0.41
3:E:410:ILE:HG23	3:E:441:PHE:CD2	2.55	0.41
1:A:94:ILE:HG22	9:A:616:HOH:O	2.19	0.41
1:A:220:LEU:HB3	1:A:226:MET:HG2	2.01	0.41
1:C:106:ARG:NH1	1:C:121:ILE:HD13	2.35	0.41
1:C:396:GLN:O	1:C:400:VAL:HG23	2.20	0.41
3:E:357:ILE:O	3:E:363:VAL:HG13	2.20	0.41
2:F:218:VAL:HG21	2:F:236:GLY:HA2	2.03	0.41
4:G:10:LEU:O	4:G:14:LYS:HG3	2.21	0.41
1:B:87:ILE:HD12	1:B:87:ILE:N	2.36	0.41
1:B:341:ASN:O	1:B:345:ILE:HG13	2.20	0.41
1:B:367:VAL:HG12	1:B:367:VAL:O	2.21	0.41
2:D:32:ILE:O	2:D:33:LEU:HB2	2.19	0.41
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.41
1:B:166:LEU:O	1:B:349:GLN:HA	2.20	0.41
1:B:389:THR:HA	1:B:392:LEU:HD12	2.02	0.41
2:D:196:LEU:HG	2:D:200:MET:CE	2.51	0.41
3:E:151:LYS:HG2	3:E:293:GLN:OE1	2.20	0.41
1:A:24:ASP:O	1:A:26:GLU:N	2.53	0.41
1:A:247:PRO:HG3	1:A:274:GLN:NE2	2.35	0.41
1:A:479:LEU:HA	1:A:482:LYS:HE2	2.02	0.41
1:B:52:MET:HG2	1:B:95:VAL:HA	2.02	0.41
1:B:410:LEU:O	1:B:411:ASP:HB3	2.20	0.41
1:C:139:ARG:NH1	1:C:310:ALA:HB2	2.36	0.41
2:F:151:LYS:HD3	2:F:328:HIS:O	2.21	0.41
1:A:132:LYS:HE3	1:A:132:LYS:HB2	1.96	0.41
1:A:148:THR:O	1:A:182:THR:HA	2.21	0.41
1:A:439:GLU:O	1:A:442:VAL:HG22	2.21	0.41
1:B:34:ILE:HD12	1:B:38:ILE:O	2.20	0.41
1:B:98:PRO:HG3	1:B:126:ARG:HH12	1.86	0.41
1:B:217:VAL:HG12	1:B:231:VAL:HG21	2.03	0.41
1:B:461:ILE:O	1:B:464:PHE:HB3	2.21	0.41
1:C:249:SER:O	1:C:253:MET:HG3	2.21	0.41
1:C:295:PRO:O	1:C:298:VAL:HG23	2.21	0.41
3:E:137:ILE:HG22	3:E:139:VAL:HG22	2.02	0.41
1:B:413:ALA:O	1:B:417:LEU:HG	2.20	0.41
2:D:186:VAL:HB	2:D:257:ASN:O	2.20	0.41
3:E:110:THR:OG1	3:E:113:PHE:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:141:ASP:O	3:E:145:PRO:HG3	2.21	0.41
3:E:409:LYS:NZ	3:E:450:ASP:HA	2.36	0.41
2:F:181:SER:HB2	2:F:215:VAL:HG22	2.02	0.41
1:A:292:GLU:O	1:A:293:ALA:HB3	2.21	0.40
1:A:400:VAL:HG12	1:A:400:VAL:O	2.21	0.40
1:B:450:ARG:HB2	1:B:452:TYR:CE2	2.56	0.40
2:F:20:VAL:HG13	2:F:59:ARG:HG3	2.03	0.40
2:F:84:ILE:HG21	2:F:235:THR:HG23	2.03	0.40
2:F:349:ASP:HA	2:F:350:PRO:HD2	1.88	0.40
1:B:220:LEU:CB	1:B:226:MET:HG2	2.48	0.40
1:B:386:VAL:HG23	1:B:387:ALA:H	1.85	0.40
2:D:93:ARG:HH21	2:D:101:PRO:HB3	1.87	0.40
1:A:356:LEU:HB3	1:A:361:ILE:HB	2.02	0.40
2:D:93:ARG:NH2	2:D:106:GLY:O	2.54	0.40
2:D:405:SER:O	2:D:409:LYS:HG3	2.21	0.40
3:E:405:SER:O	3:E:409:LYS:HG3	2.21	0.40
2:F:153:GLY:HA3	2:F:329:LEU:CD1	2.47	0.40
4:G:259:THR:O	4:G:263:ILE:HG13	2.20	0.40
1:A:300:TYR:CZ	3:E:225:PRO:HG3	2.57	0.40
2:F:137:ILE:HD12	2:F:418:PHE:CZ	2.56	0.40
2:F:312:VAL:HA	2:F:313:PRO:HD2	1.98	0.40
1:B:166:LEU:HD12	1:B:325:PRO:O	2.22	0.40
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.86	0.40
1:C:67:GLU:O	2:D:71:ARG:NH1	2.54	0.40
1:C:472:VAL:HG23	1:C:480:LEU:HD11	2.02	0.40
1:C:501:VAL:HG23	1:C:502:THR:N	2.37	0.40
2:D:406:ARG:NH2	2:D:447:GLY:HA3	2.36	0.40
4:G:24:LYS:HD2	4:G:233:ASP:HA	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	485/510 (95%)	448 (92%)	34 (7%)	3 (1%)	25	64
1	B	485/510 (95%)	436 (90%)	43 (9%)	6 (1%)	13	48
1	C	490/510 (96%)	452 (92%)	36 (7%)	2 (0%)	34	72
2	D	465/480 (97%)	409 (88%)	49 (10%)	7 (2%)	10	42
2	F	464/480 (97%)	426 (92%)	33 (7%)	5 (1%)	14	50
3	E	463/480 (96%)	428 (92%)	29 (6%)	6 (1%)	12	45
4	G	116/272 (43%)	109 (94%)	6 (5%)	1 (1%)	17	55
All	All	2968/3242 (92%)	2708 (91%)	230 (8%)	30 (1%)	15	53

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	247	GLU
3	E	451	HIS
2	F	451	HIS
1	B	69	ASP
1	B	121	ILE
1	C	25	LEU
1	C	388	GLY
2	D	393	MET
3	E	394	ASP
1	A	25	LEU
1	A	26	GLU
1	B	375	GLY
1	B	467	ALA
2	F	44	ARG
4	G	88	GLN
2	D	394	ASP
3	E	28	GLY
1	A	138	PRO
1	B	237	SER
2	D	124	VAL
2	D	395	GLU
3	E	423	VAL
2	F	124	VAL
3	E	279	VAL
2	F	220	GLY
1	B	95	VAL
3	E	390	ILE
2	F	279	VAL
2	D	140	VAL

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Mol	Chain	Res	Type
2	D	220	GLY

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	393/412 (95%)	388 (99%)	5 (1%)	69	89
1	B	393/412 (95%)	387 (98%)	6 (2%)	65	87
1	C	397/412 (96%)	391 (98%)	6 (2%)	65	87
2	D	377/384 (98%)	374 (99%)	3 (1%)	81	93
2	F	376/384 (98%)	373 (99%)	3 (1%)	81	93
3	E	375/383 (98%)	367 (98%)	8 (2%)	53	82
4	G	102/230 (44%)	100 (98%)	2 (2%)	55	83
All	All	2413/2617 (92%)	2380 (99%)	33 (1%)	67	88

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ILE
1	A	151	LYS
1	A	237	SER
1	A	406	PHE
1	A	490	SER
1	B	143	ARG
1	B	181	ASP
1	B	186	GLN
1	B	244	TYR
1	B	380	THR
1	B	414	THR
1	C	216	LEU
1	C	219	ARG
1	C	349	GLN
1	C	416	GLN
1	C	479	LEU

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Mol	Chain	Res	Type
1	C	486	ASP
2	D	67	GLU
2	D	112	GLN
2	D	282	GLN
3	E	67	GLU
3	E	132	ILE
3	E	210	ASP
3	E	252	LEU
3	E	282	GLN
3	E	352	ASP
3	E	431	LEU
3	E	455	GLN
2	F	67	GLU
2	F	282	GLN
2	F	455	GLN
4	G	77	LEU
4	G	254	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	471	HIS
1	A	475	GLN
1	B	260	ASN
1	C	46	ASN
1	C	208	GLN
1	C	260	ASN
2	D	282	GLN
3	E	282	GLN
3	E	367	HIS
3	E	455	GLN
2	F	198	HIS
2	F	223	ASN
2	F	246	GLN
2	F	282	GLN
2	F	385	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)

1 non-standard protein/DNA/RNA residue is 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	TYN	E	311	3	21,24,25	1.91	6 (28%)	21,33,35	0.62	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	TYN	E	311	3	-	2/9/16/18	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	311	TYN	C6-N2	-4.22	1.31	1.39
3	E	311	TYN	C2-C1	3.70	1.44	1.40
3	E	311	TYN	C1-N1	-3.40	1.33	1.39
3	E	311	TYN	C4-C3	3.14	1.44	1.38
3	E	311	TYN	C2-N3	2.78	1.47	1.37
3	E	311	TYN	C3-C2	-2.22	1.35	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	311	TYN	CA-CB-CG-CD1
3	E	311	TYN	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ATP	A	600	5	26,33,33	0.72	0	31,52,52	1.33	4 (12%)
6	ATP	C	600	5	26,33,33	0.79	0	31,52,52	1.29	5 (16%)
7	ADP	D	600	5	24,29,29	0.72	0	29,45,45	1.05	3 (10%)
6	ATP	F	600	5	26,33,33	0.74	0	31,52,52	1.29	4 (12%)
8	PO4	E	602	-	4,4,4	1.88	3 (75%)	6,6,6	0.41	0
6	ATP	B	600	5	26,33,33	0.74	0	31,52,52	1.30	4 (12%)

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
6	ATP	A	600	5	-	0/18/38/38	0/3/3/3
6	ATP	C	600	5	-	0/18/38/38	0/3/3/3
7	ADP	D	600	5	-	0/12/32/32	0/3/3/3
6	ATP	F	600	5	-	2/18/38/38	0/3/3/3
6	ATP	B	600	5	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	602	PO4	P-O2	-2.14	1.48	1.54
8	E	602	PO4	P-O4	-2.08	1.48	1.54
8	E	602	PO4	P-O3	-2.04	1.48	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	600	ATP	PA-O3A-PB	-3.53	120.73	132.83
6	A	600	ATP	PB-O3B-PG	-3.50	120.82	132.83
6	C	600	ATP	PB-O3B-PG	-3.44	121.02	132.83
7	D	600	ADP	PA-O3A-PB	-3.39	121.20	132.83
6	B	600	ATP	PB-O3B-PG	-3.35	121.33	132.83
6	B	600	ATP	PA-O3A-PB	-3.35	121.34	132.83
6	C	600	ATP	PA-O3A-PB	-3.34	121.38	132.83
6	A	600	ATP	PA-O3A-PB	-3.30	121.52	132.83
6	F	600	ATP	PB-O3B-PG	-3.28	121.55	132.83
6	A	600	ATP	C5-C6-N6	2.41	124.01	120.35
6	B	600	ATP	O3G-PG-O2G	2.32	116.49	107.64
6	C	600	ATP	O3G-PG-O2G	2.31	116.46	107.64
6	A	600	ATP	O3G-PG-O2G	2.29	116.40	107.64
6	B	600	ATP	C5-C6-N6	2.27	123.80	120.35
7	D	600	ADP	O2B-PB-O1B	2.25	119.50	110.68
6	F	600	ATP	O3G-PG-O2G	2.25	116.22	107.64
7	D	600	ADP	C5-C6-N6	2.20	123.70	120.35
6	F	600	ATP	C5-C6-N6	2.13	123.59	120.35
6	C	600	ATP	C5-C6-N6	2.08	123.52	120.35
6	C	600	ATP	O3B-PG-O1G	-2.02	100.01	111.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	600	ATP	PA-O3A-PB-O1B
6	F	600	ATP	PA-O3A-PB-O2B

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	ATP	2	0
6	C	600	ATP	2	0
7	D	600	ADP	1	0

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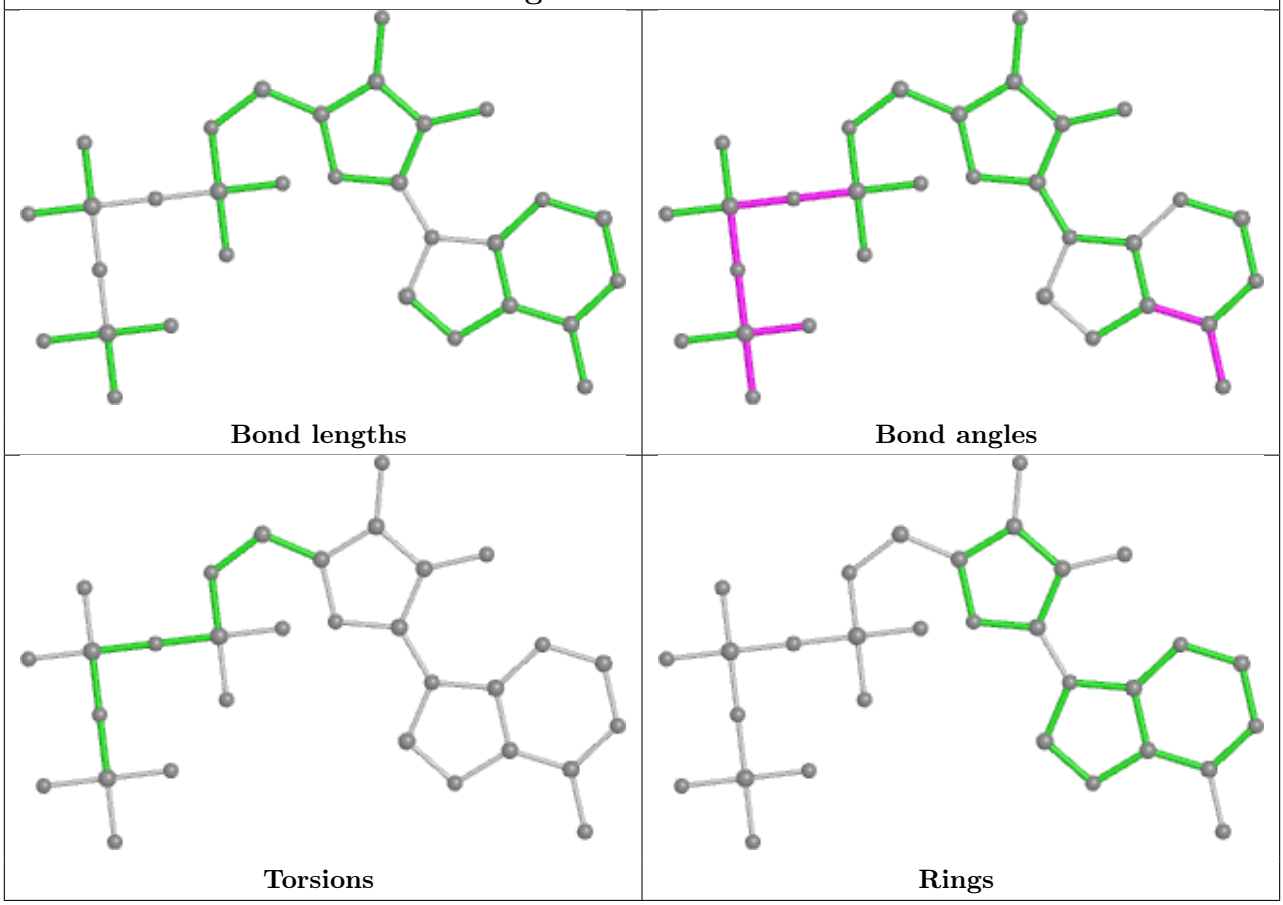
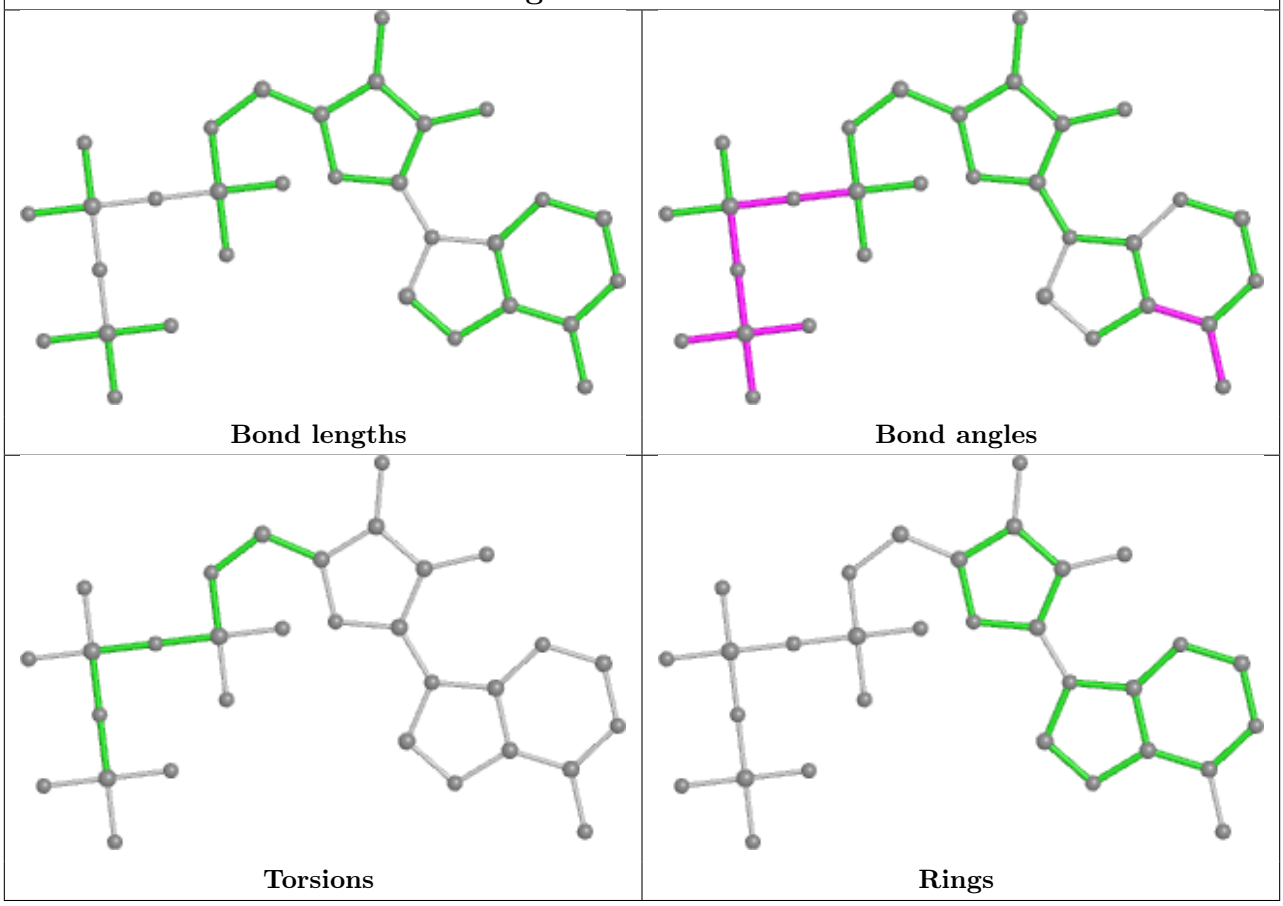
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	600	ATP	1	0
6	B	600	ATP	1	0

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.

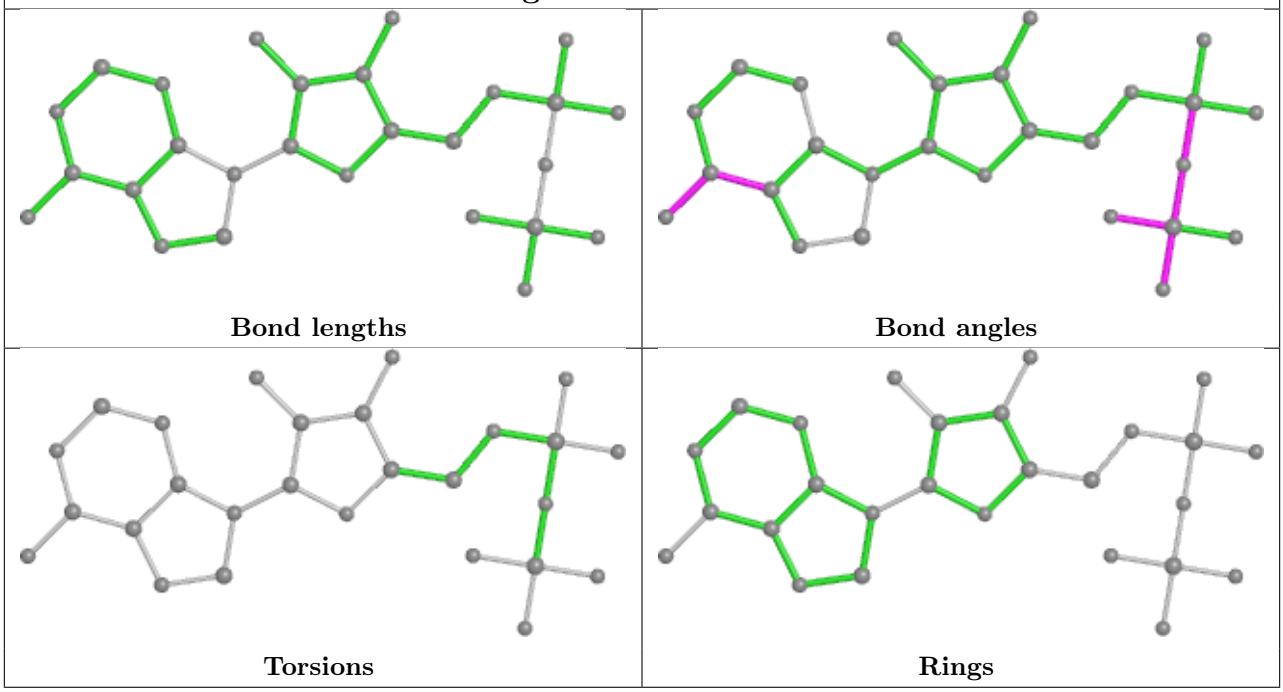
Ligand ATP A 600



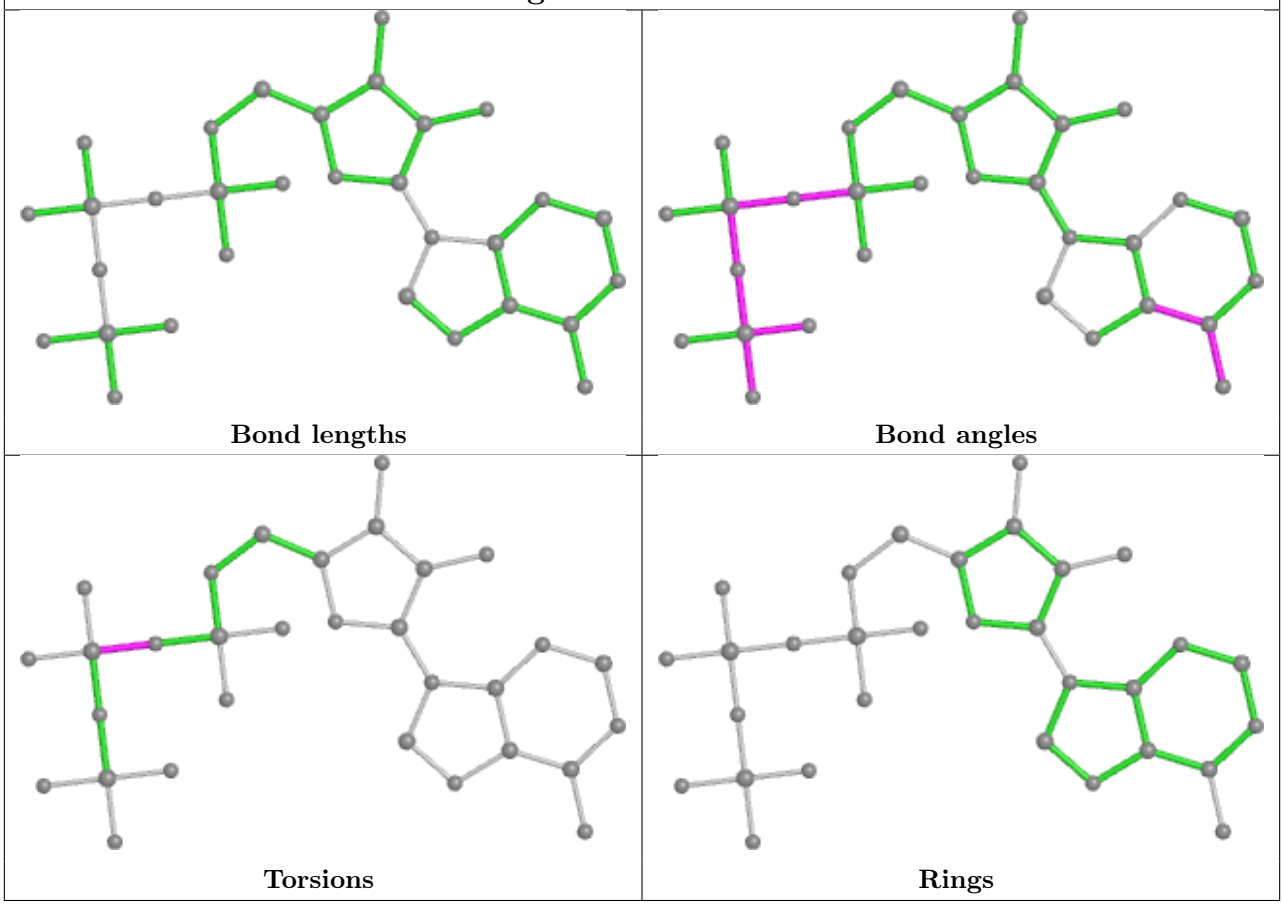
Ligand ATP C 600



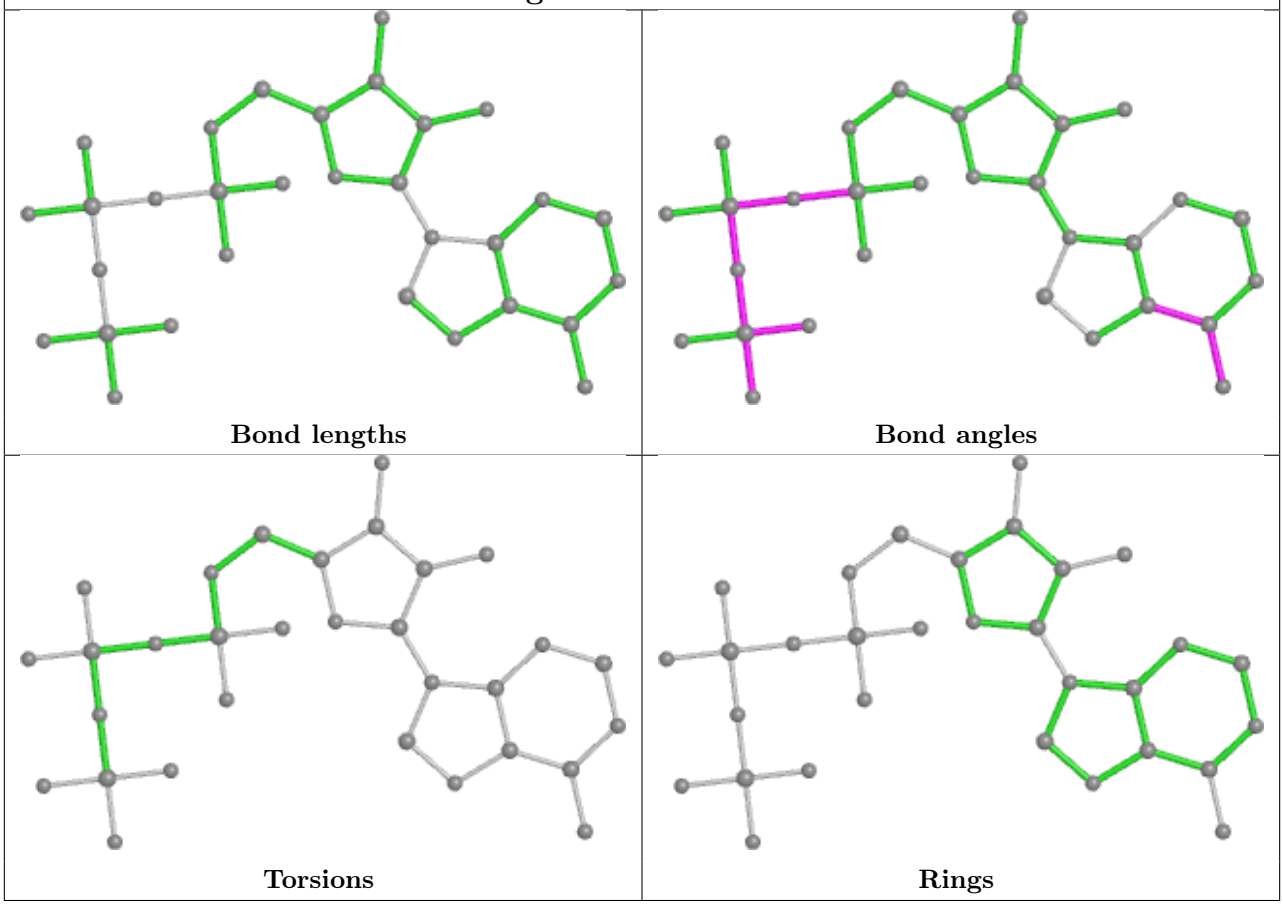
Ligand ADP D 600



Ligand ATP F 600



Ligand ATP B 600



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	487/510 (95%)	-0.48	5 (1%)	82	59	12, 52, 91, 100	0
1	B	479/510 (93%)	-0.38	11 (2%)	60	31	18, 52, 98, 100	0
1	C	492/510 (96%)	-0.43	4 (0%)	86	65	17, 50, 86, 100	0
2	D	467/480 (97%)	-0.39	6 (1%)	77	51	15, 52, 96, 100	0
2	F	466/480 (97%)	-0.49	2 (0%)	92	79	11, 47, 85, 99	0
3	E	465/480 (96%)	-0.33	7 (1%)	73	46	15, 56, 98, 100	0
4	G	122/272 (44%)	0.55	21 (17%)	1	0	18, 78, 100, 100	0
All	All	2978/3242 (91%)	-0.38	56 (1%)	66	37	11, 52, 96, 100	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	86	ALA	5.0
4	G	211	ASN	5.0
3	E	391	LEU	4.3
4	G	90	LYS	4.2
1	C	408	SER	4.1
4	G	212	ILE	4.1
4	G	41	ALA	4.1
4	G	89	MET	4.0
2	D	390	ILE	3.9
2	D	389	ALA	3.8
4	G	210	ALA	3.7
4	G	43	VAL	3.5
4	G	209	LEU	3.5
4	G	87	LYS	3.4
4	G	216	SER	3.3
1	B	120	PRO	3.3
4	G	40	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	3.3
1	C	412	ALA	3.1
3	E	473	LEU	2.9
1	B	413	ALA	2.9
1	B	396	GLN	2.9
2	D	387	ILE	2.8
2	F	210	ASP	2.7
3	E	389	ALA	2.7
4	G	88	GLN	2.6
4	G	214	TYR	2.6
4	G	213	ILE	2.6
1	A	408	SER	2.5
4	G	38	LEU	2.4
4	G	215	TYR	2.4
1	B	414	THR	2.4
3	E	110	THR	2.4
2	F	453	PRO	2.4
1	A	406	PHE	2.4
1	B	121	ILE	2.4
2	D	453	PRO	2.4
4	G	44	TYR	2.4
1	B	57	SER	2.3
4	G	220	SER	2.3
3	E	423	VAL	2.3
1	A	194	ASP	2.3
4	G	85	VAL	2.3
1	B	485	THR	2.3
1	B	457	GLU	2.2
1	C	406	PHE	2.2
1	A	143	ARG	2.1
3	E	9	THR	2.1
2	D	472	LYS	2.1
1	C	409	ASP	2.1
1	B	411	ASP	2.1
1	A	123	SER	2.1
3	E	210	ASP	2.1
1	B	400	VAL	2.0
2	D	394	ASP	2.0
4	G	42	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
3	TYN	E	311	22/23	0.91	0.20	38,98,100,100	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

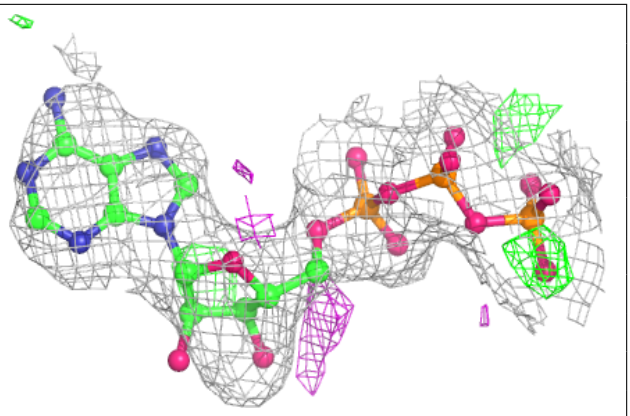
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

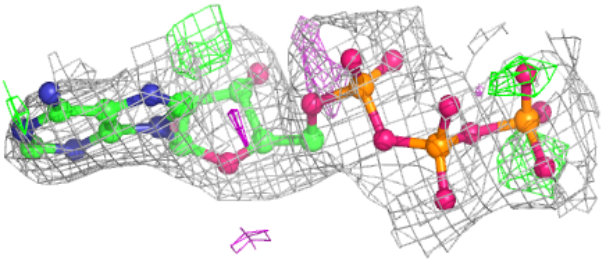
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PO4	E	602	5/5	0.66	0.36	95,100,100,100	0
5	MG	A	601	1/1	0.76	0.18	43,43,43,43	0
5	MG	C	601	1/1	0.87	0.18	51,51,51,51	0
5	MG	F	601	1/1	0.90	0.11	28,28,28,28	0
6	ATP	A	600	31/31	0.91	0.20	29,51,66,76	0
5	MG	D	601	1/1	0.91	0.25	57,57,57,57	0
6	ATP	C	600	31/31	0.93	0.17	26,44,61,79	0
6	ATP	B	600	31/31	0.93	0.17	26,49,64,68	0
5	MG	B	601	1/1	0.96	0.17	25,25,25,25	0
7	ADP	D	600	27/27	0.97	0.14	25,44,54,59	0
6	ATP	F	600	31/31	0.97	0.11	23,42,57,63	0

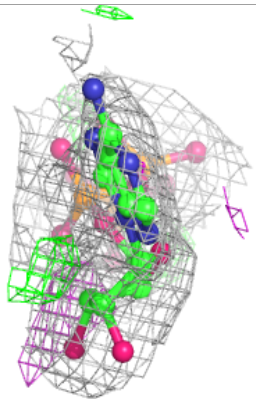
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 600:

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

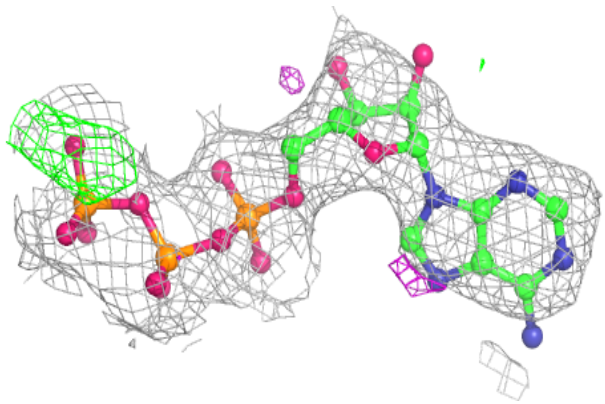


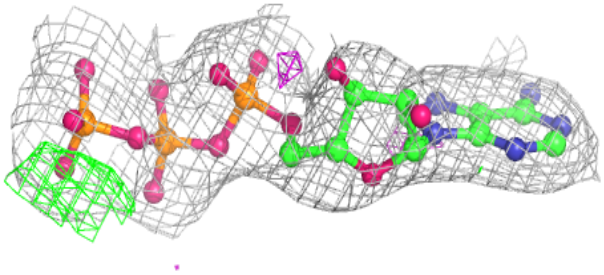


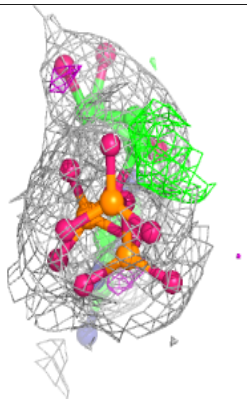


Electron density around ATP C 600:

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

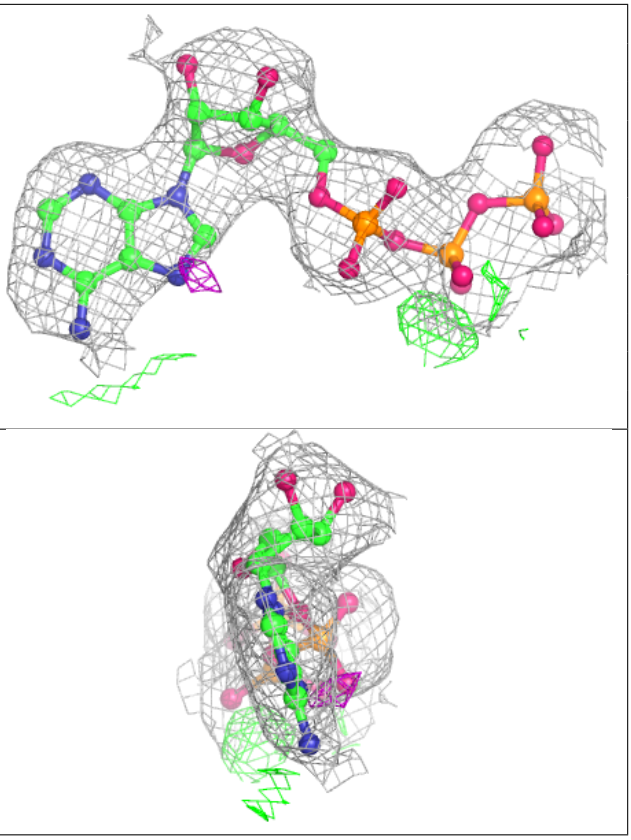


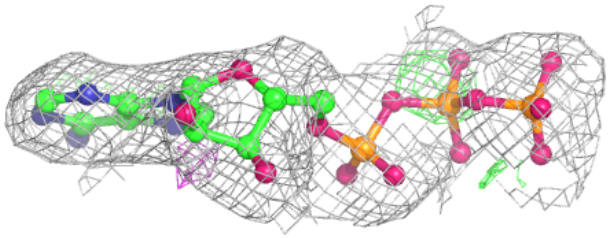




Electron density around ATP B 600:

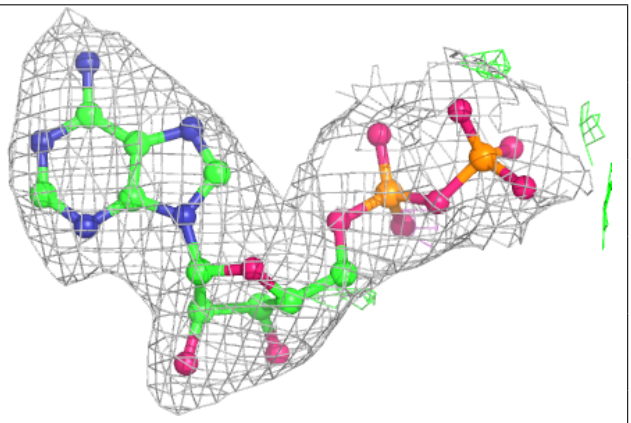
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

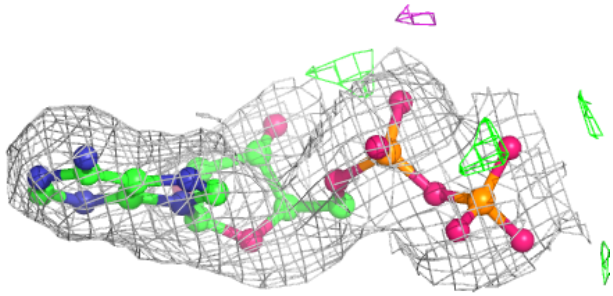


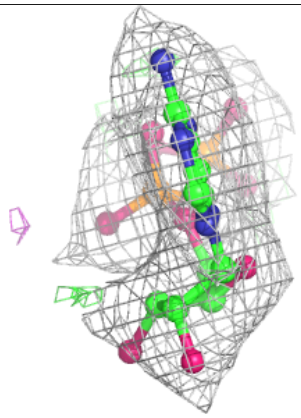


Electron density around ADP D 600:

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

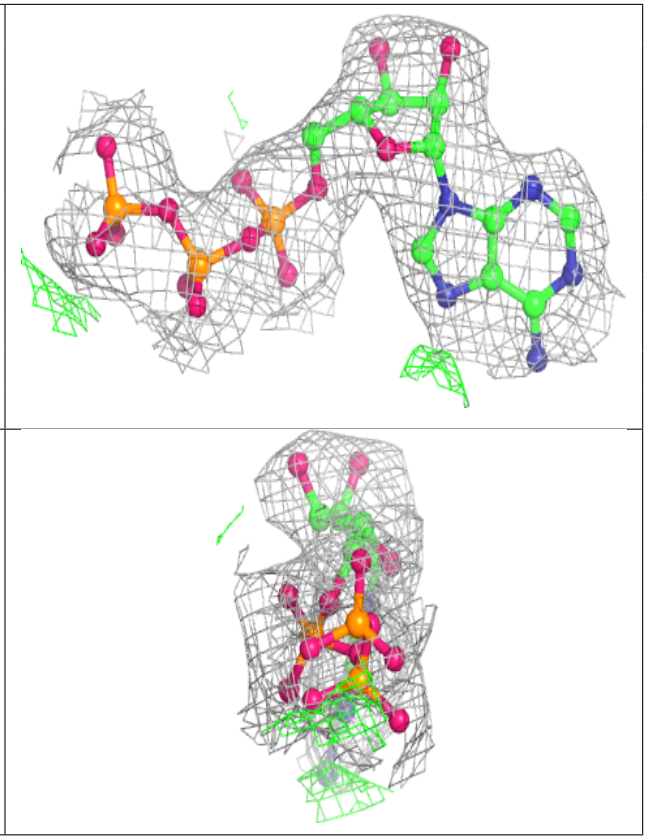






Electron density around ATP F 600:

$2mF_o$-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.