Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2022 – 06:20 pm GMT

PDB ID	:	6R72
Title	:	Crystal structure of BmrA-E504A in an outward-facing conformation
Authors	:	Chaptal, V.; Zampieri, V.; Kilburg, A.; Magnard, S.; Falson, P.
Deposited on	:	2019-03-28
Resolution	:	3.95 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 following versions of software and data (see references (i)) were used in the production of this report:

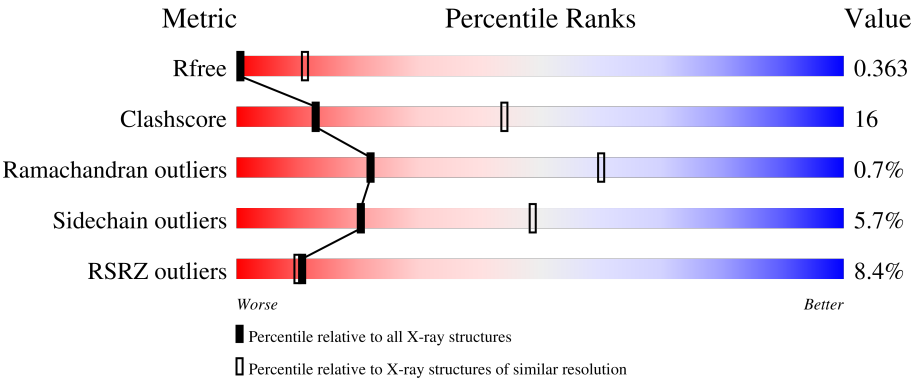
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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	599	7% 67% 26% • 5%
1	B	599	8% 66% 27% • 5%
1	C	599	9% 67% 25% • 6%
1	D	599	9% 67% 26% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17683 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 Multidrug exporter ATP-binding cassette.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4396	2822	734	823	17			
1	B	569	Total	C	N	O	S	0	0	0
			4392	2820	733	821	18			
1	C	565	Total	C	N	O	S	0	0	0
			4367	2806	728	816	17			
1	D	572	Total	C	N	O	S	0	0	0
			4400	2824	735	824	17			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A164TVX9
A	-8	SER	-	expression tag	UNP A0A164TVX9
A	-7	SER	-	expression tag	UNP A0A164TVX9
A	-6	SER	-	expression tag	UNP A0A164TVX9
A	-5	HIS	-	expression tag	UNP A0A164TVX9
A	-4	HIS	-	expression tag	UNP A0A164TVX9
A	-3	HIS	-	expression tag	UNP A0A164TVX9
A	-2	HIS	-	expression tag	UNP A0A164TVX9
A	-1	HIS	-	expression tag	UNP A0A164TVX9
A	0	HIS	-	expression tag	UNP A0A164TVX9
A	504	ALA	GLU	engineered mutation	UNP A0A164TVX9
B	-9	MET	-	initiating methionine	UNP A0A164TVX9
B	-8	SER	-	expression tag	UNP A0A164TVX9
B	-7	SER	-	expression tag	UNP A0A164TVX9
B	-6	SER	-	expression tag	UNP A0A164TVX9
B	-5	HIS	-	expression tag	UNP A0A164TVX9
B	-4	HIS	-	expression tag	UNP A0A164TVX9
B	-3	HIS	-	expression tag	UNP A0A164TVX9
B	-2	HIS	-	expression tag	UNP A0A164TVX9
B	-1	HIS	-	expression tag	UNP A0A164TVX9
B	0	HIS	-	expression tag	UNP A0A164TVX9

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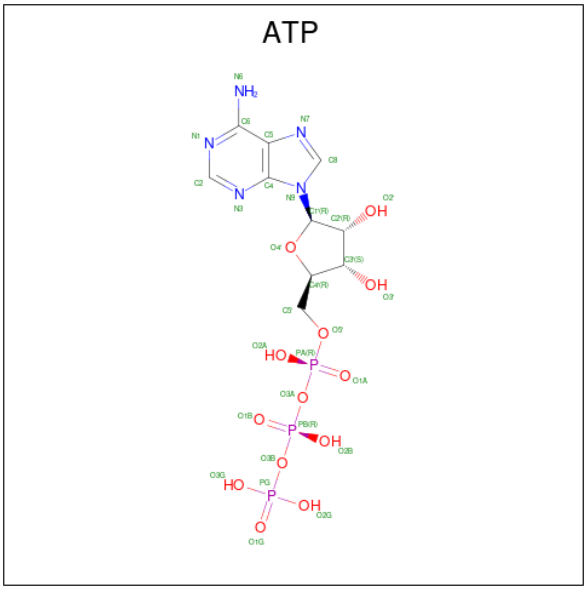
Chain	Residue	Modelled	Actual	Comment	Reference
B	504	ALA	GLU	engineered mutation	UNP A0A164TVX9
C	-9	MET	-	initiating methionine	UNP A0A164TVX9
C	-8	SER	-	expression tag	UNP A0A164TVX9
C	-7	SER	-	expression tag	UNP A0A164TVX9
C	-6	SER	-	expression tag	UNP A0A164TVX9
C	-5	HIS	-	expression tag	UNP A0A164TVX9
C	-4	HIS	-	expression tag	UNP A0A164TVX9
C	-3	HIS	-	expression tag	UNP A0A164TVX9
C	-2	HIS	-	expression tag	UNP A0A164TVX9
C	-1	HIS	-	expression tag	UNP A0A164TVX9
C	0	HIS	-	expression tag	UNP A0A164TVX9
C	504	ALA	GLU	engineered mutation	UNP A0A164TVX9
D	-9	MET	-	initiating methionine	UNP A0A164TVX9
D	-8	SER	-	expression tag	UNP A0A164TVX9
D	-7	SER	-	expression tag	UNP A0A164TVX9
D	-6	SER	-	expression tag	UNP A0A164TVX9
D	-5	HIS	-	expression tag	UNP A0A164TVX9
D	-4	HIS	-	expression tag	UNP A0A164TVX9
D	-3	HIS	-	expression tag	UNP A0A164TVX9
D	-2	HIS	-	expression tag	UNP A0A164TVX9
D	-1	HIS	-	expression tag	UNP A0A164TVX9
D	0	HIS	-	expression tag	UNP A0A164TVX9
D	504	ALA	GLU	engineered mutation	UNP A0A164TVX9

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

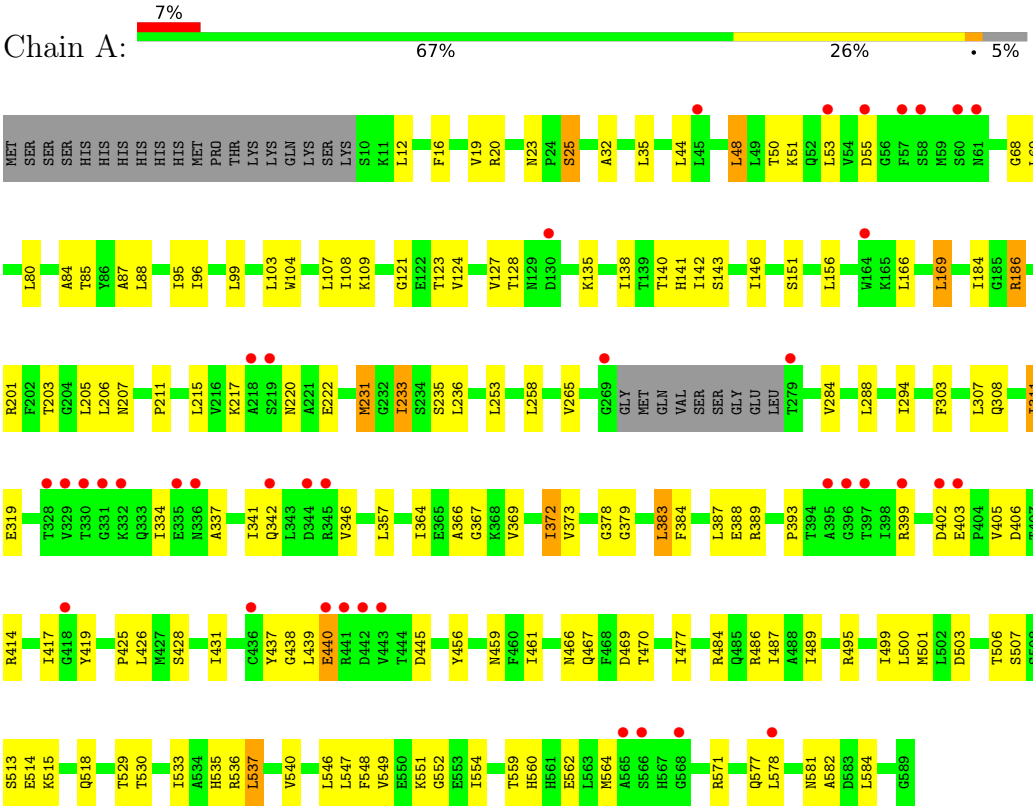
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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.

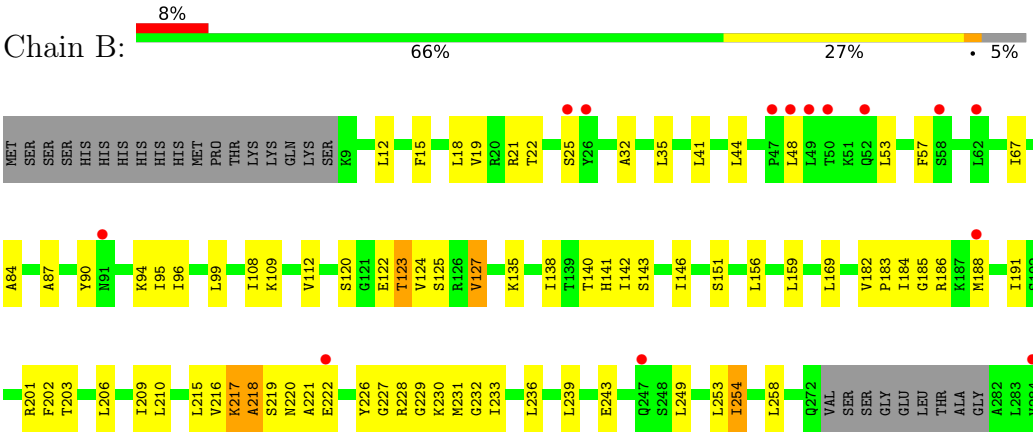
• Molecule 1: Multidrug exporter ATP-binding cassette

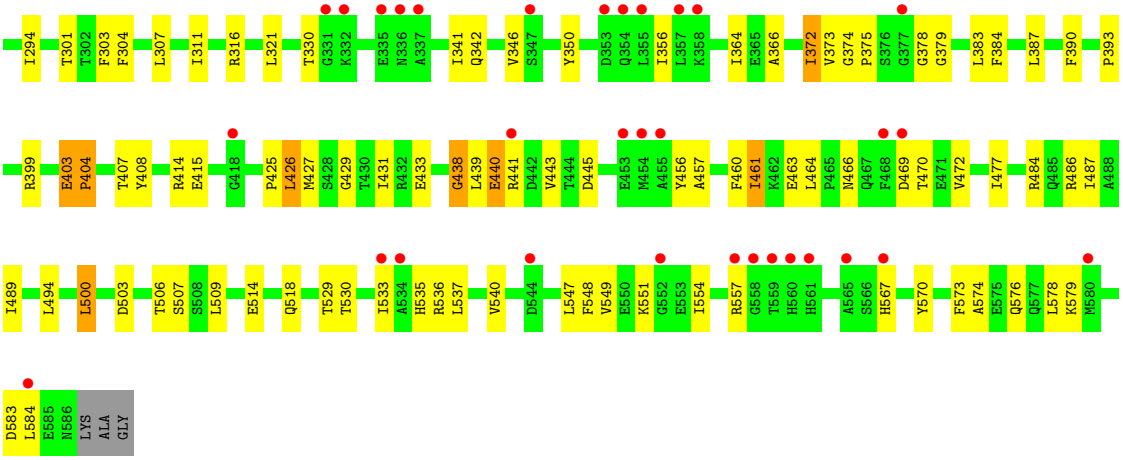
Chain A:



• Molecule 1: Multidrug exporter ATP-binding cassette

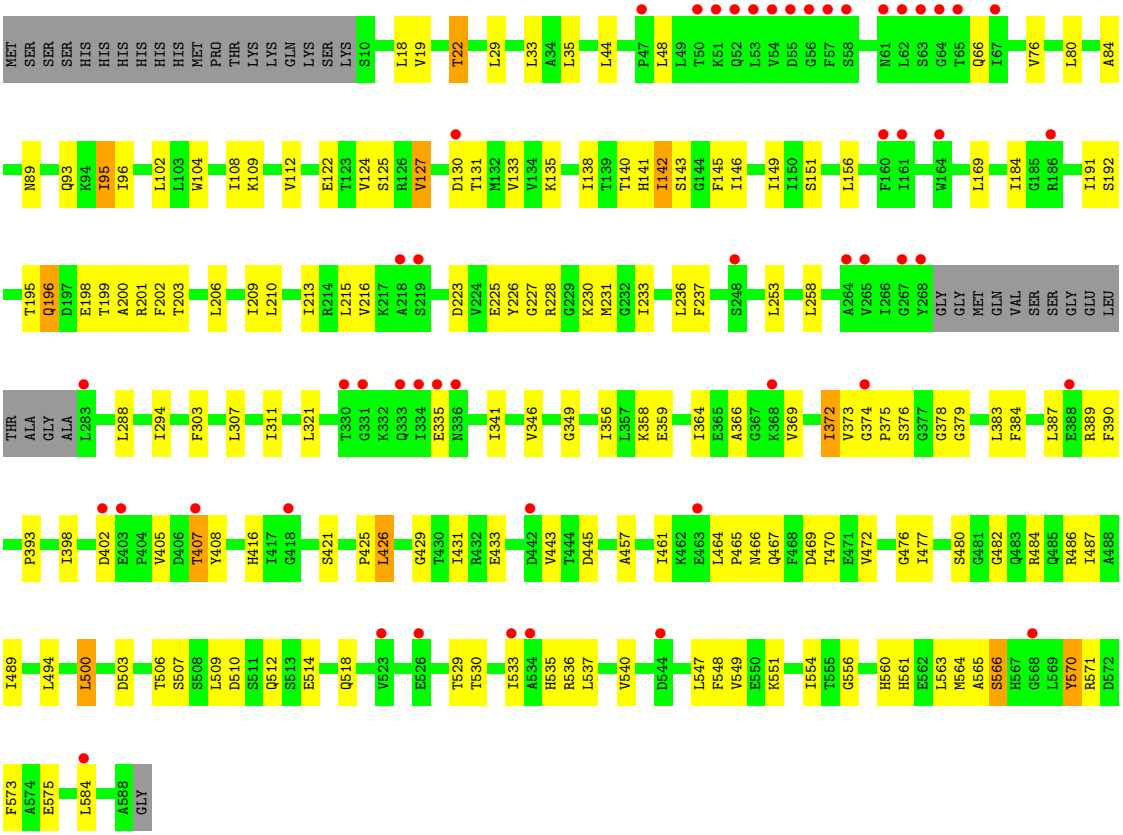
Chain B:





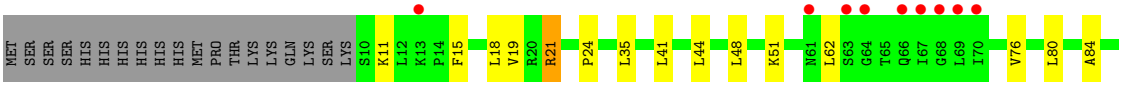
• Molecule 1: Multidrug exporter ATP-binding cassette

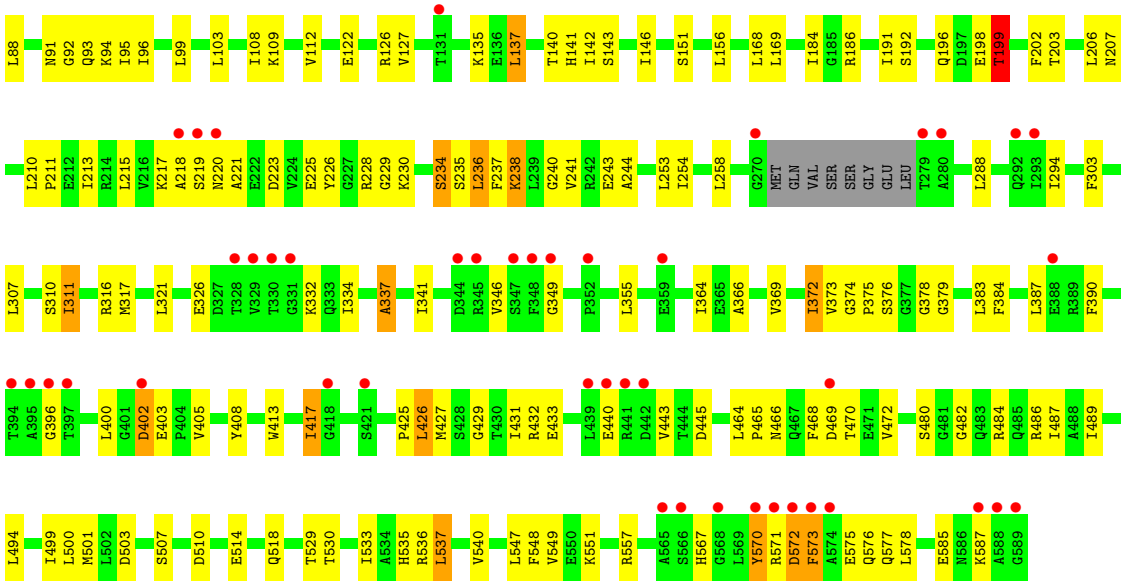
Chain C:



• Molecule 1: Multidrug exporter ATP-binding cassette

Chain D:




L88 N91 G92 Q93 K94 I95 I96 L99 L103 I108 K109 V112 E122 R126 V127 T131 K135 E136 L137 T140 H141 I142 S143 I146 S151 L156 L168 L169 I184 G185 R186 I191 S192 Q196 D197 E198 T199 F202 T203 L206 N207
L210 P211 E212 I213 R214 L215 V216 K217 A218 S219 N220 A221 E222 D223 V224 E225 Y226 G227 R228 G229 K230 S234 S235 L236 F237 K238 L239 G240 V241 R242 E243 A244 L253 I254 L258 G270 MET GLN VAL SER SER GLY GLU LEU T279 A280 L288 Q292 I293 I294 F303
L307 S310 I311 R316 M317 L321 E326 D327 T328 V329 T330 G331 K332 Q333 I334 A337 I341 D344 R345 V346 S347 F348 G349 P352 L355 E359 I364 E365 A366 V369 I372 V373 G374 P375 S376 G377 G378 G379 L383 F384 L387 E388 R389 F390
T394 A395 G396 T397 L400 G401 D402 E403 P404 V405 Y408 W413 I417 G418 S421 P425 L426 M427 S428 G429 T430 I431 R432 E433 L439 E440 R441 D442 V443 T444 D445 L464 P465 N466 Q467 F468 D469 T470 E471 V472 S480 G481 G482 Q483 R484 Q485 R486 I487 A488 I489
L494 I499 L500 M501 L502 D503 S507 D510 E514 Q518 T529 T530 I533 A534 H535 R536 L537 V540 L547 F548 V549 E550 K551 R557 A565 S566 H567 G568 L569 Y570 R571 D572 F573 A574 E575 Q576 Q577 L578 E585 N586 K587 A588 G589

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.81Å 110.75Å 155.62Å 90.00° 93.23° 90.00°	Depositor
Resolution (Å)	28.42 – 3.95 28.42 – 3.95	Depositor EDS
% Data completeness (in resolution range)	92.0 (28.42-3.95) 57.9 (28.42-3.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.98Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.260 , 0.321 0.299 , 0.363	Depositor DCC
R_{free} test set	1019 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	198.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	17683	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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, 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	0.44	0/4462	0.80	15/6038 (0.2%)
1	B	0.44	0/4458	0.77	10/6031 (0.2%)
1	C	0.45	0/4433	0.77	8/5999 (0.1%)
1	D	0.45	0/4466	0.79	17/6043 (0.3%)
All	All	0.45	0/17819	0.78	50/24111 (0.2%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	337	ALA	CB-CA-C	15.17	132.86	110.10
1	A	408	TYR	N-CA-C	-14.04	73.10	111.00
1	B	438	GLY	N-CA-C	13.63	147.17	113.10
1	C	566	SER	N-CA-C	12.03	143.49	111.00
1	B	439	LEU	CB-CA-C	-11.80	87.78	110.20
1	A	402	ASP	CB-CA-C	-11.38	87.64	110.40
1	A	439	LEU	CB-CA-C	-11.31	88.71	110.20
1	C	566	SER	N-CA-CB	-10.61	94.59	110.50
1	B	440	GLU	N-CA-CB	-10.54	91.63	110.60
1	C	402	ASP	CB-CA-C	-10.09	90.22	110.40
1	A	551	LYS	CB-CA-C	-9.85	90.70	110.40
1	A	409	SER	N-CA-CB	-9.34	96.49	110.50
1	A	440	GLU	N-CA-CB	-9.25	93.95	110.60
1	D	551	LYS	CB-CA-C	-9.06	92.28	110.40
1	C	551	LYS	CB-CA-C	-8.89	92.63	110.40
1	D	402	ASP	CB-CA-C	-8.85	92.69	110.40
1	C	565	ALA	CB-CA-C	-8.85	96.83	110.10
1	B	551	LYS	CB-CA-C	-8.37	93.65	110.40
1	A	409	SER	CB-CA-C	8.19	125.66	110.10
1	B	439	LEU	N-CA-C	-7.80	89.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	379	GLY	N-CA-C	7.66	132.26	113.10
1	B	441	ARG	CB-CA-C	-7.62	95.16	110.40
1	A	403	GLU	N-CA-CB	7.47	124.05	110.60
1	D	573	PHE	N-CA-CB	7.44	123.99	110.60
1	B	379	GLY	N-CA-C	7.32	131.41	113.10
1	C	379	GLY	N-CA-C	7.31	131.37	113.10
1	A	379	GLY	N-CA-C	7.25	131.23	113.10
1	D	572	ASP	CB-CA-C	6.88	124.17	110.40
1	D	572	ASP	N-CA-C	-6.73	92.83	111.00
1	D	218	ALA	CB-CA-C	6.67	120.10	110.10
1	A	403	GLU	N-CA-C	-6.41	93.70	111.00
1	D	238	LYS	N-CA-CB	6.29	121.92	110.60
1	D	403	GLU	N-CA-CB	6.26	121.86	110.60
1	D	219	SER	N-CA-C	6.04	127.30	111.00
1	B	218	ALA	N-CA-C	-6.02	94.75	111.00
1	A	231	MET	CB-CA-C	5.91	122.23	110.40
1	D	202	PHE	CB-CA-C	5.84	122.08	110.40
1	B	219	SER	CB-CA-C	-5.82	99.03	110.10
1	A	317	MET	N-CA-CB	5.73	120.92	110.60
1	C	565	ALA	N-CA-C	5.59	126.10	111.00
1	D	326	GLU	N-CA-C	5.58	126.07	111.00
1	D	137	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	552	GLY	N-CA-C	5.25	126.22	113.10
1	A	55	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	203	THR	CB-CA-C	-5.14	97.72	111.60
1	A	439	LEU	N-CA-CB	5.05	120.50	110.40
1	D	236	LEU	N-CA-C	5.05	124.63	111.00
1	C	570	TYR	CB-CA-C	-5.03	100.34	110.40
1	D	199	THR	CB-CA-C	-5.03	98.03	111.60
1	B	440	GLU	N-CA-C	5.02	124.56	111.00

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	4396	0	4566	181	0
1	B	4392	0	4562	147	0
1	C	4367	0	4539	171	0
1	D	4400	0	4568	156	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	17683	0	18283	590	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 16.

All (590) 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:D:141:HIS:CD2	1:D:303:PHE:CE1	1.93	1.53
1:C:141:HIS:CD2	1:C:303:PHE:CE1	2.13	1.35
1:A:217:LYS:HD2	1:B:414:ARG:NH1	1.40	1.35
1:A:141:HIS:CD2	1:A:303:PHE:CE1	2.15	1.33
1:D:99:LEU:HD22	1:D:317:MET:SD	1.68	1.33
1:A:99:LEU:HD22	1:A:317:MET:SD	1.69	1.33
1:D:198:GLU:HB3	1:D:236:LEU:CD1	1.60	1.32
1:D:141:HIS:HD2	1:D:303:PHE:CD1	1.48	1.30
1:C:198:GLU:OE2	1:C:236:LEU:HD13	1.30	1.29
1:A:217:LYS:HD3	1:A:222:GLU:OE2	1.21	1.28
1:C:141:HIS:CD2	1:C:303:PHE:HE1	1.50	1.26
1:C:104:TRP:CH2	1:D:206:LEU:HD21	1.75	1.22
1:B:141:HIS:CD2	1:B:303:PHE:CE1	2.27	1.21
1:D:141:HIS:CD2	1:D:303:PHE:HE1	1.38	1.21
1:D:198:GLU:HB3	1:D:236:LEU:HD12	1.20	1.19
1:A:388:GLU:CG	1:A:419:TYR:CD2	2.27	1.17
1:D:198:GLU:CB	1:D:236:LEU:HD13	1.75	1.17
1:B:184:ILE:HD11	1:B:253:LEU:HD22	1.24	1.14
1:D:184:ILE:HD11	1:D:253:LEU:CD1	1.78	1.13
1:A:141:HIS:HD2	1:A:303:PHE:CD1	1.66	1.12
1:B:141:HIS:CD2	1:B:303:PHE:HE1	1.65	1.11
1:C:184:ILE:HD11	1:C:253:LEU:CD1	1.79	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLU:OE1	1:B:236:LEU:HD22	1.49	1.09
1:A:103:LEU:HD21	1:A:317:MET:HG3	1.32	1.09
1:D:19:VAL:CG2	1:D:95:ILE:HD11	1.81	1.09
1:A:35:LEU:HD12	1:A:84:ALA:HB2	1.31	1.09
1:A:99:LEU:CD2	1:A:317:MET:HE1	1.82	1.09
1:A:99:LEU:HD23	1:A:317:MET:HE1	1.19	1.09
1:D:141:HIS:NE2	1:D:303:PHE:CE1	2.21	1.08
1:C:141:HIS:HD2	1:C:303:PHE:CD1	1.72	1.07
1:D:198:GLU:CB	1:D:236:LEU:CD1	2.33	1.06
1:C:226:TYR:O	1:C:230:LYS:HB3	1.56	1.06
1:D:238:LYS:O	1:D:241:VAL:HG23	1.54	1.06
1:B:249:LEU:O	1:B:253:LEU:HD13	1.55	1.05
1:C:509:LEU:CD2	1:C:514:GLU:HB2	1.85	1.05
1:C:200:ALA:O	1:C:203:THR:OG1	1.75	1.04
1:C:563:LEU:HG	1:C:570:TYR:HE2	1.20	1.04
1:D:198:GLU:CG	1:D:236:LEU:HD13	1.88	1.04
1:A:388:GLU:HG2	1:A:419:TYR:CD2	1.90	1.04
1:A:509:LEU:CD2	1:A:514:GLU:HB2	1.87	1.04
1:B:35:LEU:HD12	1:B:84:ALA:HB2	1.34	1.04
1:C:195:THR:HG23	1:C:196:GLN:NE2	1.71	1.04
1:B:184:ILE:HD11	1:B:253:LEU:CD2	1.87	1.03
1:A:141:HIS:CD2	1:A:303:PHE:HE1	1.59	1.03
1:B:229:GLY:O	1:B:233:ILE:HG22	1.57	1.03
1:D:35:LEU:HD12	1:D:84:ALA:HB2	1.42	1.01
1:C:35:LEU:HD12	1:C:84:ALA:HB2	1.38	1.01
1:A:510:ASP:OD2	1:B:375:PRO:HA	1.58	1.01
1:C:141:HIS:HD2	1:C:303:PHE:CE1	1.66	1.01
1:A:99:LEU:CD2	1:A:317:MET:CE	2.38	1.00
1:D:19:VAL:HG22	1:D:95:ILE:CD1	1.90	1.00
1:A:388:GLU:OE2	1:A:419:TYR:HD2	1.44	0.99
1:D:184:ILE:HD11	1:D:253:LEU:HD13	1.44	0.99
1:A:367:GLY:H	1:A:529:THR:CG2	1.76	0.98
1:C:198:GLU:OE2	1:C:236:LEU:CD1	2.11	0.98
1:A:217:LYS:HD2	1:B:414:ARG:HH12	1.21	0.97
1:C:192:SER:C	1:C:195:THR:HG22	1.84	0.97
1:D:141:HIS:CD2	1:D:303:PHE:CD1	2.35	0.97
1:A:141:HIS:NE2	1:A:303:PHE:CE1	2.33	0.96
1:C:184:ILE:HD11	1:C:253:LEU:HD13	1.48	0.95
1:A:217:LYS:CD	1:A:222:GLU:OE2	2.15	0.95
1:D:199:THR:HG22	1:D:237:PHE:CE1	2.01	0.95
1:A:141:HIS:CD2	1:A:303:PHE:CD1	2.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:HIS:HD2	1:B:303:PHE:CE1	1.82	0.94
1:A:367:GLY:H	1:A:529:THR:HG23	1.30	0.94
1:C:226:TYR:CZ	1:C:230:LYS:HD3	2.01	0.94
1:C:237:PHE:HD1	1:D:93:GLN:HE22	0.97	0.93
1:C:93:GLN:NE2	1:D:237:PHE:O	2.01	0.93
1:D:19:VAL:HG22	1:D:95:ILE:HD11	0.93	0.93
1:C:226:TYR:CE2	1:C:230:LYS:HD3	2.02	0.93
1:D:465:PRO:O	1:D:470:THR:HG23	1.68	0.93
1:B:198:GLU:OE1	1:B:236:LEU:CD2	2.16	0.93
1:D:198:GLU:HG3	1:D:236:LEU:HD13	1.50	0.93
1:A:99:LEU:HD22	1:A:317:MET:CE	1.99	0.92
1:C:198:GLU:OE1	1:C:202:PHE:CE1	2.22	0.92
1:B:141:HIS:HD2	1:B:303:PHE:CD1	1.86	0.92
1:C:465:PRO:O	1:C:470:THR:HG23	1.69	0.92
1:A:509:LEU:HD22	1:A:514:GLU:HB2	1.49	0.92
1:A:217:LYS:HD2	1:B:414:ARG:HH11	1.27	0.92
1:D:141:HIS:NE2	1:D:303:PHE:HE1	1.64	0.91
1:A:99:LEU:HD23	1:A:317:MET:CE	1.99	0.91
1:C:192:SER:HA	1:C:195:THR:CG2	2.00	0.90
1:C:199:THR:O	1:C:203:THR:HG23	1.71	0.90
1:B:193:ARG:HD3	1:B:316:ARG:HH22	1.35	0.89
1:D:199:THR:HG22	1:D:237:PHE:CZ	2.08	0.88
1:D:238:LYS:O	1:D:241:VAL:CG2	2.20	0.88
1:A:99:LEU:CD2	1:A:317:MET:SD	2.61	0.88
1:B:193:ARG:HD3	1:B:316:ARG:NH2	1.89	0.88
1:A:217:LYS:CD	1:B:414:ARG:NH1	2.33	0.88
1:A:366:ALA:HA	1:A:529:THR:CG2	2.03	0.88
1:A:437:TYR:CE2	1:B:220:ASN:ND2	2.42	0.88
1:B:229:GLY:O	1:B:233:ILE:CG2	2.22	0.87
1:C:109:LYS:HA	1:D:217:LYS:HZ1	1.36	0.87
1:A:206:LEU:HD11	1:B:124:VAL:HG13	1.58	0.86
1:B:90:TYR:CZ	1:B:94:LYS:HD2	2.11	0.86
1:C:237:PHE:HD1	1:D:93:GLN:NE2	1.73	0.86
1:A:184:ILE:HD11	1:A:253:LEU:HD13	1.58	0.86
1:A:388:GLU:HG3	1:A:419:TYR:CD2	2.09	0.86
1:A:388:GLU:OE2	1:A:419:TYR:CD2	2.28	0.85
1:A:141:HIS:NE2	1:A:303:PHE:HE1	1.72	0.85
1:C:509:LEU:HD21	1:C:514:GLU:CA	2.06	0.85
1:C:563:LEU:HG	1:C:570:TYR:CE2	2.11	0.85
1:A:437:TYR:CD2	1:B:220:ASN:ND2	2.45	0.84
1:C:192:SER:CA	1:C:195:THR:HG22	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:GLU:O	1:C:202:PHE:HD1	1.61	0.84
1:C:104:TRP:CZ2	1:D:206:LEU:HD21	2.13	0.83
1:C:104:TRP:CH2	1:D:206:LEU:CD2	2.60	0.83
1:C:141:HIS:NE2	1:C:303:PHE:CE1	2.45	0.83
1:B:227:GLY:O	1:B:231:MET:HG2	1.79	0.83
1:C:509:LEU:CD2	1:C:514:GLU:CB	2.56	0.83
1:D:99:LEU:CD2	1:D:317:MET:SD	2.60	0.83
1:D:378:GLY:O	1:D:549:VAL:HG12	1.78	0.83
1:B:76:VAL:O	1:B:80:LEU:HG	1.79	0.82
1:B:125:SER:OG	1:B:203:THR:HG21	1.78	0.82
1:C:563:LEU:CG	1:C:570:TYR:HE2	1.92	0.82
1:C:192:SER:O	1:C:195:THR:CG2	2.27	0.82
1:A:76:VAL:O	1:A:80:LEU:HG	1.79	0.82
1:C:76:VAL:O	1:C:80:LEU:HG	1.79	0.81
1:C:509:LEU:HD22	1:C:514:GLU:HB2	1.62	0.81
1:D:400:LEU:CD1	1:D:413:TRP:HE1	1.93	0.81
1:A:217:LYS:CD	1:B:414:ARG:HH12	1.91	0.81
1:C:108:ILE:O	1:D:217:LYS:HD3	1.80	0.81
1:A:231:MET:O	1:A:235:SER:HB3	1.80	0.80
1:B:184:ILE:CD1	1:B:253:LEU:HD22	2.08	0.80
1:D:206:LEU:HD13	1:D:206:LEU:O	1.81	0.80
1:A:509:LEU:HD22	1:A:514:GLU:CB	2.12	0.80
1:A:206:LEU:CD1	1:B:124:VAL:HG13	2.12	0.79
1:C:192:SER:O	1:C:195:THR:HG22	1.81	0.79
1:D:103:LEU:HD21	1:D:317:MET:HG3	1.63	0.79
1:A:509:LEU:CD2	1:A:514:GLU:CB	2.60	0.79
1:A:231:MET:O	1:A:235:SER:CB	2.31	0.79
1:C:192:SER:HA	1:C:195:THR:HG21	1.62	0.79
1:C:374:GLY:O	1:D:510:ASP:OD2	2.00	0.79
1:D:76:VAL:O	1:D:80:LEU:HG	1.82	0.79
1:C:510:ASP:OD2	1:D:375:PRO:HA	1.83	0.78
1:D:141:HIS:HD2	1:D:303:PHE:HD1	1.30	0.78
1:B:90:TYR:O	1:B:94:LYS:HG3	1.83	0.78
1:A:509:LEU:HD21	1:A:514:GLU:CA	2.12	0.78
1:A:509:LEU:HD21	1:A:514:GLU:N	1.97	0.78
1:A:201:ARG:O	1:A:205:LEU:HG	1.84	0.77
1:C:509:LEU:HD21	1:C:514:GLU:HA	1.66	0.77
1:A:378:GLY:O	1:A:549:VAL:HG12	1.83	0.77
1:C:506:THR:HG22	1:C:509:LEU:HD13	1.67	0.77
1:D:198:GLU:CG	1:D:236:LEU:CD1	2.62	0.76
1:C:426:LEU:HD11	1:C:484:ARG:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:GLU:O	1:B:440:GLU:HG3	1.86	0.75
1:D:225:GLU:OE1	1:D:228:ARG:HD2	1.86	0.75
1:C:466:ASN:HB2	1:C:469:ASP:HB2	1.66	0.75
1:B:188:MET:CE	1:B:243:GLU:OE2	2.35	0.75
1:A:103:LEU:CD2	1:A:317:MET:HG3	2.16	0.75
1:A:388:GLU:CD	1:A:419:TYR:HD2	1.90	0.75
1:C:108:ILE:O	1:D:217:LYS:NZ	2.18	0.75
1:D:184:ILE:CD1	1:D:253:LEU:CD1	2.64	0.75
1:A:103:LEU:HD11	1:A:317:MET:SD	2.26	0.74
1:B:53:LEU:HB3	1:B:57:PHE:CZ	2.21	0.74
1:C:104:TRP:CZ3	1:D:206:LEU:HD21	2.22	0.74
1:A:388:GLU:HG2	1:A:419:TYR:CG	2.23	0.73
1:D:207:ASN:O	1:D:211:PRO:HD3	1.88	0.73
1:C:22:THR:HB	1:C:102:LEU:HD11	1.69	0.73
1:C:195:THR:CG2	1:C:196:GLN:NE2	2.50	0.73
1:B:426:LEU:HD11	1:B:484:ARG:HB2	1.69	0.73
1:C:141:HIS:NE2	1:C:303:PHE:HE1	1.80	0.73
1:C:378:GLY:O	1:C:549:VAL:HG12	1.89	0.73
1:A:437:TYR:HD2	1:B:220:ASN:HD22	1.31	0.72
1:B:216:VAL:O	1:B:220:ASN:OD1	2.07	0.72
1:C:509:LEU:HD23	1:C:514:GLU:HB2	1.71	0.72
1:B:226:TYR:CZ	1:B:230:LYS:HD3	2.24	0.72
1:B:188:MET:HE1	1:B:243:GLU:OE2	1.90	0.72
1:C:184:ILE:CD1	1:C:253:LEU:CD1	2.65	0.72
1:A:141:HIS:HD2	1:A:303:PHE:HD1	1.36	0.72
1:C:192:SER:HA	1:C:195:THR:HG22	1.67	0.72
1:C:209:ILE:HD11	1:C:228:ARG:HH22	1.54	0.72
1:A:388:GLU:HG3	1:A:419:TYR:CE2	2.26	0.71
1:B:25:SER:OG	1:B:94:LYS:HE2	1.89	0.71
1:B:378:GLY:O	1:B:549:VAL:HG12	1.91	0.71
1:B:141:HIS:NE2	1:B:303:PHE:CE1	2.59	0.71
1:A:203:THR:O	1:A:206:LEU:HG	1.91	0.70
1:C:184:ILE:HD11	1:C:253:LEU:HD12	1.74	0.70
1:C:226:TYR:CZ	1:C:230:LYS:CD	2.74	0.70
1:D:11:LYS:HD2	1:D:186:ARG:HH12	1.57	0.70
1:C:509:LEU:HD22	1:C:514:GLU:CB	2.21	0.70
1:A:35:LEU:CD1	1:A:84:ALA:HB2	2.17	0.70
1:A:509:LEU:HD23	1:A:510:ASP:O	1.92	0.70
1:C:141:HIS:CD2	1:C:303:PHE:CD1	2.59	0.70
1:A:367:GLY:H	1:A:529:THR:HG22	1.57	0.69
1:C:196:GLN:OE1	1:C:196:GLN:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:TYR:HE1	1:A:459:ASN:HD22	1.40	0.69
1:D:228:ARG:HG3	1:D:229:GLY:N	2.06	0.69
1:D:225:GLU:OE2	1:D:228:ARG:NE	2.25	0.69
1:D:184:ILE:HD11	1:D:253:LEU:HD12	1.73	0.69
1:A:388:GLU:CG	1:A:419:TYR:HD2	1.99	0.69
1:D:466:ASN:HB2	1:D:469:ASP:HB3	1.74	0.69
1:C:19:VAL:HG13	1:C:95:ILE:HD11	1.76	0.68
1:C:509:LEU:CD2	1:C:514:GLU:CA	2.71	0.68
1:A:509:LEU:CD2	1:A:514:GLU:CA	2.70	0.68
1:D:226:TYR:O	1:D:230:LYS:CB	2.41	0.68
1:A:103:LEU:HD21	1:A:317:MET:CG	2.19	0.68
1:A:388:GLU:CD	1:A:419:TYR:CD2	2.64	0.68
1:C:109:LYS:HA	1:D:217:LYS:NZ	2.09	0.68
1:D:240:GLY:O	1:D:243:GLU:N	2.26	0.68
1:A:366:ALA:HA	1:A:529:THR:HG21	1.76	0.67
1:C:349:GLY:HA2	1:C:356:ILE:HG22	1.77	0.67
1:B:141:HIS:NE2	1:B:303:PHE:HE1	1.92	0.66
1:A:388:GLU:OE2	1:A:419:TYR:HB3	1.96	0.66
1:B:226:TYR:CE2	1:B:230:LYS:HD3	2.31	0.66
1:C:561:HIS:HB3	1:D:587:LYS:HE2	1.78	0.66
1:A:316:ARG:HA	1:A:319:GLU:HG2	1.78	0.66
1:C:226:TYR:O	1:C:230:LYS:CB	2.40	0.66
1:D:35:LEU:CD1	1:D:84:ALA:HB2	2.22	0.66
1:D:226:TYR:O	1:D:230:LYS:HB2	1.95	0.66
1:C:192:SER:CA	1:C:195:THR:CG2	2.69	0.66
1:A:207:ASN:OD1	1:B:124:VAL:HG21	1.96	0.65
1:A:284:VAL:HG11	1:B:57:PHE:CE1	2.31	0.65
1:C:407:THR:CG2	1:C:408:TYR:N	2.58	0.65
1:A:367:GLY:N	1:A:529:THR:CG2	2.55	0.65
1:B:431:ILE:HD13	1:B:461:ILE:HG13	1.78	0.65
1:B:35:LEU:CD1	1:B:84:ALA:HB2	2.20	0.65
1:D:225:GLU:OE2	1:D:228:ARG:CZ	2.45	0.65
1:A:426:LEU:HD21	1:A:484:ARG:HB2	1.80	0.64
1:D:141:HIS:NE2	1:D:307:LEU:HD13	2.11	0.64
1:C:142:ILE:O	1:C:146:ILE:HG12	1.97	0.64
1:C:510:ASP:OD2	1:D:374:GLY:O	2.15	0.64
1:A:124:VAL:O	1:A:127:VAL:HG12	1.98	0.64
1:A:512:GLN:HG3	1:B:576:GLN:HG3	1.80	0.64
1:D:91:ASN:O	1:D:95:ILE:HG22	1.98	0.63
1:C:506:THR:HG21	1:C:514:GLU:HG2	1.81	0.63
1:A:406:ASP:O	1:A:408:TYR:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:ILE:HD13	1:C:467:GLN:HE21	1.64	0.63
1:C:507:SER:HB2	1:D:507:SER:HB2	1.81	0.62
1:D:206:LEU:HD13	1:D:206:LEU:C	2.19	0.62
1:A:431:ILE:HD13	1:A:461:ILE:HG12	1.80	0.62
1:B:373:VAL:O	1:B:548:PHE:HA	2.00	0.62
1:D:341:ILE:HA	1:D:400:LEU:HD23	1.82	0.62
1:A:217:LYS:HG3	1:A:217:LYS:O	1.99	0.62
1:B:141:HIS:CD2	1:B:303:PHE:CD1	2.70	0.62
1:B:141:HIS:HE2	1:B:307:LEU:HD13	1.65	0.62
1:C:227:GLY:O	1:C:231:MET:HB2	1.99	0.61
1:C:198:GLU:OE2	1:C:236:LEU:HD22	2.00	0.61
1:B:138:ILE:HD12	1:B:141:HIS:ND1	2.15	0.61
1:C:509:LEU:HD21	1:C:514:GLU:N	2.16	0.61
1:A:389:ARG:NH1	1:A:405:VAL:HG22	2.16	0.61
1:A:184:ILE:CD1	1:A:253:LEU:HD13	2.30	0.61
1:A:367:GLY:N	1:A:529:THR:HG23	2.11	0.60
1:D:137:LEU:HD21	1:D:310:SER:HB3	1.83	0.60
1:D:184:ILE:CD1	1:D:253:LEU:HD12	2.29	0.60
1:C:104:TRP:CZ2	1:D:206:LEU:CD2	2.84	0.60
1:D:112:VAL:HG21	1:D:390:PHE:HB3	1.83	0.60
1:A:103:LEU:HD11	1:A:317:MET:HG3	1.82	0.60
1:A:206:LEU:HD23	1:A:233:ILE:CD1	2.32	0.60
1:C:198:GLU:OE1	1:C:202:PHE:HE1	1.77	0.60
1:B:567:HIS:HB2	1:B:570:TYR:HD1	1.67	0.60
1:B:112:VAL:HG21	1:B:390:PHE:HB3	1.83	0.59
1:C:112:VAL:HG21	1:C:390:PHE:HB3	1.84	0.59
1:D:99:LEU:HD22	1:D:317:MET:CE	2.31	0.59
1:A:509:LEU:HD23	1:A:514:GLU:HB2	1.82	0.59
1:B:429:GLY:HA3	1:B:433:GLU:OE1	2.01	0.59
1:C:35:LEU:CD1	1:C:84:ALA:HB2	2.22	0.59
1:D:24:PRO:HD2	1:D:94:LYS:HG2	1.83	0.59
1:C:184:ILE:CD1	1:C:253:LEU:HD12	2.30	0.59
1:C:141:HIS:HE2	1:C:307:LEU:HD13	1.67	0.59
1:C:192:SER:O	1:C:195:THR:HG23	2.01	0.59
1:D:199:THR:CG2	1:D:237:PHE:CE1	2.82	0.59
1:D:429:GLY:HA3	1:D:433:GLU:OE1	2.03	0.59
1:B:574:ALA:HB1	1:B:578:LEU:HD12	1.84	0.59
1:C:375:PRO:HA	1:D:510:ASP:OD2	2.03	0.58
1:A:509:LEU:HD21	1:A:514:GLU:HA	1.85	0.58
1:C:225:GLU:OE1	1:C:228:ARG:NH2	2.31	0.58
1:B:404:PRO:HD2	1:B:407:THR:OG1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:O	1:C:213:ILE:HG23	2.02	0.58
1:A:499:ILE:HG12	1:A:529:THR:OG1	2.03	0.58
1:D:225:GLU:OE1	1:D:228:ARG:CD	2.51	0.58
1:A:510:ASP:OD2	1:B:375:PRO:CA	2.43	0.58
1:C:122:GLU:HG3	1:C:201:ARG:HG3	1.86	0.58
1:C:206:LEU:HD21	1:C:233:ILE:HD11	1.84	0.58
1:A:515:LYS:HZ3	1:B:579:LYS:HD3	1.68	0.57
1:B:403:GLU:HB3	1:B:408:TYR:HB2	1.84	0.57
1:B:464:LEU:HB3	1:B:470:THR:HG21	1.85	0.57
1:C:108:ILE:O	1:D:217:LYS:CD	2.50	0.57
1:C:512:GLN:HG3	1:D:576:GLN:HG3	1.86	0.57
1:A:367:GLY:N	1:A:529:THR:HG22	2.18	0.57
1:B:90:TYR:CE2	1:B:94:LYS:HD2	2.39	0.57
1:A:103:LEU:HD11	1:A:317:MET:CG	2.35	0.57
1:D:486:ARG:HA	1:D:489:ILE:HD12	1.87	0.57
1:A:220:ASN:HA	1:B:414:ARG:HH21	1.70	0.57
1:B:188:MET:HE3	1:B:243:GLU:OE2	2.05	0.57
1:D:213:ILE:HG13	1:D:217:LYS:HG2	1.86	0.57
1:B:547:LEU:HD23	1:B:557:ARG:HG2	1.85	0.57
1:A:316:ARG:HA	1:A:319:GLU:CG	2.34	0.57
1:A:581:ASN:HB2	1:A:584:LEU:HD12	1.87	0.57
1:C:96:ILE:HD12	1:C:135:LYS:HB2	1.86	0.57
1:A:389:ARG:NH1	1:A:405:VAL:O	2.38	0.56
1:A:96:ILE:HD12	1:A:135:LYS:HB2	1.86	0.56
1:A:231:MET:O	1:A:235:SER:OG	2.24	0.56
1:B:466:ASN:HB2	1:B:469:ASP:HB2	1.86	0.56
1:A:25:SER:OG	1:A:95:ILE:HD11	2.05	0.56
1:C:198:GLU:OE1	1:C:202:PHE:CZ	2.57	0.56
1:C:372:ILE:HG13	1:C:547:LEU:HB2	1.88	0.56
1:A:141:HIS:HE2	1:A:307:LEU:HD13	1.70	0.56
1:A:284:VAL:HG11	1:B:57:PHE:CD1	2.41	0.56
1:D:96:ILE:HD12	1:D:135:LYS:HB2	1.87	0.56
1:D:571:ARG:O	1:D:572:ASP:C	2.44	0.56
1:B:90:TYR:CE1	1:B:94:LYS:HD2	2.40	0.56
1:A:19:VAL:O	1:A:23:ASN:HB2	2.05	0.56
1:B:22:THR:HG21	1:B:99:LEU:HG	1.87	0.56
1:B:372:ILE:HG13	1:B:547:LEU:HB2	1.88	0.56
1:C:429:GLY:HA3	1:C:433:GLU:OE1	2.04	0.56
1:D:432:ARG:HD2	1:D:468:PHE:HB3	1.87	0.56
1:D:426:LEU:HD21	1:D:484:ARG:HB2	1.88	0.56
1:B:230:LYS:HA	1:B:233:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:TYR:O	1:C:570:TYR:CD2	2.58	0.56
1:C:138:ILE:HD12	1:C:141:HIS:ND1	2.21	0.55
1:C:512:GLN:HA	1:D:576:GLN:HE21	1.72	0.55
1:A:431:ILE:CD1	1:A:470:THR:OG1	2.54	0.55
1:B:125:SER:OG	1:B:203:THR:CG2	2.54	0.55
1:C:563:LEU:CD2	1:C:570:TYR:CE2	2.89	0.55
1:A:104:TRP:NE1	1:B:229:GLY:HA3	2.21	0.55
1:C:130:ASP:HA	1:C:133:VAL:HG23	1.89	0.55
1:D:103:LEU:HD11	1:D:317:MET:HG3	1.88	0.55
1:B:229:GLY:O	1:B:233:ILE:CB	2.55	0.55
1:A:372:ILE:HG13	1:A:547:LEU:HB2	1.89	0.55
1:B:96:ILE:HD12	1:B:135:LYS:HB2	1.89	0.55
1:C:192:SER:C	1:C:195:THR:CG2	2.64	0.55
1:C:425:PRO:HG3	1:D:215:LEU:HD22	1.87	0.54
1:C:563:LEU:CD2	1:C:570:TYR:HE2	2.19	0.54
1:A:486:ARG:HA	1:A:489:ILE:HD12	1.90	0.54
1:D:547:LEU:HD23	1:D:557:ARG:HG2	1.90	0.54
1:C:472:VAL:HG12	1:C:476:GLY:HA2	1.90	0.54
1:D:228:ARG:CG	1:D:229:GLY:N	2.70	0.54
1:A:220:ASN:O	1:B:438:GLY:O	2.25	0.54
1:C:535:HIS:CD2	1:C:536:ARG:HG2	2.43	0.54
1:D:372:ILE:HG13	1:D:547:LEU:HB2	1.88	0.54
1:C:141:HIS:NE2	1:C:307:LEU:HD13	2.22	0.54
1:A:438:GLY:HA3	1:A:495:ARG:HD3	1.90	0.53
1:A:509:LEU:HD21	1:A:513:SER:C	2.28	0.53
1:A:535:HIS:CD2	1:A:536:ARG:HG2	2.43	0.53
1:A:141:HIS:NE2	1:A:307:LEU:HD13	2.24	0.53
1:B:32:ALA:HB2	1:B:87:ALA:HB3	1.90	0.53
1:B:535:HIS:CD2	1:B:536:ARG:HG2	2.44	0.53
1:C:457:ALA:HB2	1:C:486:ARG:HB3	1.89	0.53
1:A:578:LEU:HD21	1:B:584:LEU:HB2	1.92	0.53
1:B:503:ASP:HA	1:B:533:ILE:HB	1.91	0.53
1:B:141:HIS:NE2	1:B:307:LEU:HD13	2.24	0.52
1:C:564:MET:O	1:C:571:ARG:CA	2.57	0.52
1:C:431:ILE:HD13	1:C:461:ILE:HG12	1.92	0.52
1:D:503:ASP:HA	1:D:533:ILE:HB	1.91	0.52
1:A:32:ALA:HB2	1:A:87:ALA:HB3	1.91	0.52
1:D:141:HIS:HE2	1:D:307:LEU:HD13	1.72	0.52
1:D:238:LYS:O	1:D:241:VAL:CB	2.57	0.52
1:B:120:SER:O	1:B:123:THR:HG22	2.09	0.52
1:A:16:PHE:O	1:A:20:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HH21	1:A:308:GLN:HE22	1.57	0.52
1:C:108:ILE:O	1:D:217:LYS:CE	2.58	0.52
1:A:206:LEU:HD23	1:A:233:ILE:HD13	1.92	0.52
1:C:500:LEU:HB3	1:C:530:THR:HG23	1.91	0.52
1:C:564:MET:O	1:C:571:ARG:HB2	2.10	0.52
1:D:198:GLU:HG3	1:D:236:LEU:CD1	2.32	0.52
1:D:571:ARG:O	1:D:573:PHE:HD1	1.92	0.52
1:A:503:ASP:HA	1:A:533:ILE:HB	1.91	0.52
1:D:99:LEU:CD2	1:D:317:MET:CE	2.88	0.52
1:D:535:HIS:CD2	1:D:536:ARG:HG2	2.45	0.51
1:A:499:ILE:CG1	1:A:529:THR:OG1	2.58	0.51
1:C:503:ASP:HA	1:C:533:ILE:HB	1.92	0.51
1:C:563:LEU:CG	1:C:570:TYR:CE2	2.82	0.51
1:A:220:ASN:HB3	1:B:438:GLY:O	2.10	0.51
1:C:198:GLU:OE2	1:C:236:LEU:CD2	2.59	0.51
1:D:236:LEU:HD23	1:D:236:LEU:N	2.26	0.51
1:D:341:ILE:HB	1:D:364:ILE:HB	1.93	0.51
1:A:417:ILE:HG12	1:A:499:ILE:HB	1.93	0.51
1:B:341:ILE:HB	1:B:364:ILE:HB	1.93	0.51
1:C:563:LEU:O	1:C:566:SER:OG	2.27	0.51
1:C:198:GLU:OE2	1:C:236:LEU:CG	2.58	0.51
1:C:198:GLU:CD	1:C:202:PHE:CE1	2.84	0.51
1:C:556:GLY:HA3	1:C:563:LEU:HD11	1.93	0.51
1:B:342:GLN:HB2	1:B:399:ARG:HB2	1.92	0.51
1:C:509:LEU:HD23	1:C:510:ASP:O	2.10	0.51
1:A:231:MET:C	1:A:235:SER:HB3	2.30	0.50
1:A:341:ILE:HB	1:A:364:ILE:HB	1.93	0.50
1:C:341:ILE:HB	1:C:364:ILE:HB	1.92	0.50
1:C:560:HIS:NE2	1:C:564:MET:SD	2.84	0.50
2:C:700:ATP:H5'1	1:D:480:SER:HB3	1.93	0.50
1:A:500:LEU:HD23	1:A:501:MET:N	2.26	0.50
1:B:122:GLU:HG3	1:B:201:ARG:HG3	1.92	0.50
1:A:12:LEU:HD23	1:A:311:ILE:HD13	1.93	0.50
1:A:334:ILE:HG13	1:A:337:ALA:HB3	1.94	0.50
1:A:414:ARG:HD3	1:B:218:ALA:HA	1.93	0.50
1:D:234:SER:O	1:D:235:SER:C	2.46	0.50
1:C:198:GLU:CD	1:C:236:LEU:HD13	2.23	0.50
1:B:231:MET:HG3	1:B:232:GLY:N	2.26	0.50
1:D:217:LYS:HD2	1:D:221:ALA:HB2	1.91	0.50
1:A:456:TYR:CG	1:A:456:TYR:O	2.65	0.50
1:A:507:SER:HB2	1:B:507:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:THR:HG22	1:C:408:TYR:N	2.24	0.50
1:B:18:LEU:HD11	1:B:321:LEU:HD13	1.94	0.49
1:C:407:THR:HG22	1:C:408:TYR:H	1.77	0.49
1:D:141:HIS:CE1	1:D:307:LEU:HD13	2.47	0.49
1:D:225:GLU:OE2	1:D:228:ARG:NH1	2.45	0.49
1:A:456:TYR:O	1:A:456:TYR:CD2	2.66	0.49
1:B:500:LEU:HB3	1:B:530:THR:HG23	1.94	0.49
1:D:500:LEU:HD23	1:D:501:MET:N	2.27	0.49
1:A:107:LEU:HB3	1:B:210:LEU:HD21	1.94	0.49
1:B:460:PHE:HD1	1:B:463:GLU:HG3	1.77	0.49
1:C:560:HIS:C	1:C:560:HIS:CD2	2.85	0.49
1:C:358:LYS:O	1:C:359:GLU:C	2.51	0.49
1:C:421:SER:HB2	1:D:215:LEU:HD21	1.94	0.49
1:C:509:LEU:CD2	1:C:514:GLU:HA	2.38	0.49
1:D:44:LEU:HD11	1:D:151:SER:HA	1.95	0.49
1:B:108:ILE:HD12	1:B:109:LYS:HG3	1.95	0.48
1:B:236:LEU:HD23	1:B:239:LEU:HD11	1.95	0.48
1:B:486:ARG:HA	1:B:489:ILE:HD12	1.95	0.48
1:C:564:MET:O	1:C:571:ARG:CB	2.61	0.48
1:A:366:ALA:HA	1:A:529:THR:HG22	1.90	0.48
1:A:48:LEU:HA	1:A:51:LYS:HE3	1.95	0.48
1:A:203:THR:HA	1:A:206:LEU:CD2	2.43	0.48
1:D:464:LEU:HB3	1:D:470:THR:HG21	1.95	0.48
1:A:546:LEU:HD12	1:A:559:THR:HA	1.96	0.48
1:B:159:LEU:HD11	1:B:289:TYR:HB3	1.95	0.48
1:D:427:MET:O	1:D:472:VAL:CG2	2.62	0.48
1:A:166:LEU:HD22	1:A:265:VAL:HA	1.95	0.48
1:A:461:ILE:HD13	1:A:467:GLN:HE21	1.78	0.48
1:B:25:SER:CB	1:B:94:LYS:HE2	2.44	0.48
1:B:229:GLY:O	1:B:233:ILE:HB	2.13	0.48
1:C:564:MET:O	1:C:571:ARG:HA	2.14	0.48
1:B:216:VAL:HG12	1:B:221:ALA:HB2	1.95	0.48
1:C:124:VAL:HG22	1:D:210:LEU:HD13	1.94	0.48
1:C:570:TYR:CD1	1:C:573:PHE:HB2	2.48	0.48
1:D:369:VAL:HG13	1:D:530:THR:HB	1.96	0.48
1:D:225:GLU:CD	1:D:228:ARG:NE	2.68	0.48
1:B:12:LEU:HD22	1:B:307:LEU:HD23	1.96	0.47
1:D:93:GLN:O	1:D:93:GLN:HG3	2.13	0.47
1:A:425:PRO:HG3	1:B:215:LEU:HD22	1.95	0.47
1:A:387:LEU:C	1:A:389:ARG:H	2.17	0.47
1:A:437:TYR:HE2	1:B:220:ASN:ND2	2.04	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:ASN:HB2	1:D:469:ASP:CB	2.41	0.47
1:A:389:ARG:HH11	1:A:405:VAL:HG22	1.79	0.47
1:B:217:LYS:HA	1:B:221:ALA:HB3	1.96	0.47
1:C:398:ILE:O	1:C:405:VAL:HG13	2.15	0.47
1:D:220:ASN:HB3	1:D:223:ASP:HB3	1.96	0.47
1:B:12:LEU:HD22	1:B:307:LEU:CD2	2.44	0.47
1:C:44:LEU:HD11	1:C:151:SER:HA	1.96	0.47
1:C:124:VAL:HG21	1:D:207:ASN:ND2	2.29	0.47
1:C:215:LEU:HG	1:D:425:PRO:HG3	1.96	0.47
1:C:226:TYR:CE2	1:C:230:LYS:CD	2.89	0.47
1:A:127:VAL:HG13	1:A:128:THR:N	2.30	0.47
1:A:207:ASN:HB2	1:B:124:VAL:HG11	1.96	0.47
1:C:366:ALA:HA	1:C:529:THR:OG1	2.14	0.47
1:A:466:ASN:HB2	1:A:469:ASP:HB2	1.96	0.47
1:B:366:ALA:HA	1:B:529:THR:OG1	2.15	0.47
1:C:369:VAL:HG13	1:C:530:THR:HB	1.98	0.47
1:C:195:THR:CG2	1:C:196:GLN:HE22	2.28	0.46
1:A:198:GLU:HB3	1:A:236:LEU:HD13	1.97	0.46
1:B:537:LEU:HD13	1:B:573:PHE:HB3	1.95	0.46
1:C:480:SER:HB3	2:D:700:ATP:H5'1	1.97	0.46
1:A:44:LEU:HD11	1:A:151:SER:HA	1.97	0.46
1:D:366:ALA:HA	1:D:529:THR:OG1	2.15	0.46
1:D:108:ILE:HD12	1:D:109:LYS:HG3	1.97	0.46
1:A:500:LEU:HB3	1:A:530:THR:HG23	1.98	0.46
1:B:15:PHE:CZ	1:B:18:LEU:HD22	2.50	0.46
1:D:500:LEU:HB3	1:D:530:THR:HG23	1.98	0.46
1:A:564:MET:HA	1:A:571:ARG:HG2	1.97	0.46
1:B:125:SER:C	1:B:127:VAL:H	2.19	0.46
1:C:89:ASN:HB3	1:D:244:ALA:HB1	1.97	0.46
1:A:217:LYS:O	1:A:217:LYS:CG	2.64	0.46
1:A:369:VAL:HG13	1:A:530:THR:HB	1.97	0.46
1:A:466:ASN:O	1:A:470:THR:CG2	2.64	0.46
1:C:29:LEU:O	1:C:33:LEU:HG	2.15	0.46
1:D:537:LEU:H	1:D:577:GLN:HE22	1.64	0.46
1:B:466:ASN:CG	1:B:469:ASP:OD2	2.54	0.46
1:B:427:MET:O	1:B:472:VAL:CG2	2.64	0.46
1:C:125:SER:C	1:C:127:VAL:H	2.18	0.46
1:A:456:TYR:HE1	1:A:459:ASN:ND2	2.10	0.45
1:C:108:ILE:HD12	1:C:109:LYS:HG3	1.97	0.45
1:C:373:VAL:O	1:C:548:PHE:HA	2.16	0.45
1:D:417:ILE:HG13	1:D:499:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLN:HB2	1:A:399:ARG:HB2	1.98	0.45
1:A:316:ARG:HA	1:A:319:GLU:CD	2.37	0.45
1:B:125:SER:CB	1:B:203:THR:HG21	2.46	0.45
1:C:335:GLU:HA	1:C:416:HIS:HD2	1.82	0.45
1:A:127:VAL:HG13	1:A:128:THR:H	1.82	0.45
1:D:93:GLN:HA	1:D:96:ILE:HG22	1.99	0.45
1:D:92:GLY:HA2	1:D:95:ILE:HG22	1.98	0.45
1:C:443:VAL:HG11	1:C:494:LEU:HD11	1.98	0.45
1:C:482:GLY:HA3	1:D:376:SER:HB2	1.97	0.45
1:D:88:LEU:HD13	1:D:143:SER:HB2	1.99	0.45
1:A:215:LEU:HD13	1:B:425:PRO:HB3	1.98	0.45
1:A:510:ASP:OD2	1:B:374:GLY:O	2.34	0.45
1:B:350:TYR:HD1	1:B:356:ILE:HD13	1.82	0.45
1:B:537:LEU:O	1:B:537:LEU:HD23	2.17	0.45
1:C:547:LEU:HD22	1:C:554:ILE:HD13	1.98	0.45
1:A:140:THR:HA	1:A:143:SER:HB3	1.98	0.45
1:B:140:THR:HA	1:B:143:SER:HB3	1.99	0.45
1:B:198:GLU:OE1	1:B:236:LEU:HD21	2.11	0.45
1:C:384:PHE:HA	1:C:387:LEU:HB2	1.99	0.44
1:C:464:LEU:HB3	1:C:470:THR:HG21	1.99	0.44
1:A:85:THR:HA	1:A:88:LEU:HD12	1.99	0.44
1:B:25:SER:OG	1:B:94:LYS:CE	2.61	0.44
1:B:44:LEU:HD11	1:B:151:SER:HA	1.98	0.44
1:C:104:TRP:CZ3	1:D:206:LEU:HD11	2.53	0.44
1:D:226:TYR:O	1:D:230:LYS:HB3	2.16	0.44
1:C:140:THR:HA	1:C:143:SER:HB3	1.98	0.44
1:D:373:VAL:O	1:D:548:PHE:HA	2.18	0.44
1:A:108:ILE:HD12	1:A:109:LYS:HG3	1.99	0.44
1:A:384:PHE:HA	1:A:387:LEU:HB2	1.99	0.44
1:D:140:THR:HA	1:D:143:SER:HB3	1.98	0.44
1:A:431:ILE:HD12	1:A:470:THR:OG1	2.16	0.44
1:D:349:GLY:HA3	1:D:355:LEU:HA	1.99	0.44
1:B:209:ILE:HD11	1:B:228:ARG:HH12	1.83	0.44
1:C:195:THR:HG23	1:C:196:GLN:N	2.32	0.44
1:C:376:SER:HB2	1:D:482:GLY:HA3	2.00	0.44
1:A:357:LEU:HD11	1:A:383:LEU:HD12	1.99	0.43
1:D:24:PRO:HB2	1:D:94:LYS:HE3	1.99	0.43
1:A:506:THR:HG21	1:A:514:GLU:HG2	1.99	0.43
1:A:509:LEU:CD2	1:A:514:GLU:HA	2.43	0.43
1:B:209:ILE:HD11	1:B:228:ARG:NH1	2.33	0.43
1:C:407:THR:HG23	1:C:408:TYR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:LEU:HD21	1:B:537:LEU:CD2	2.48	0.43
1:D:346:VAL:HA	1:D:396:GLY:HA3	2.00	0.43
1:A:414:ARG:HH21	1:A:417:ILE:HG22	1.83	0.43
1:A:456:TYR:CE1	1:A:459:ASN:ND2	2.87	0.43
1:B:202:PHE:N	1:B:202:PHE:CD1	2.86	0.43
1:D:575:GLU:HA	1:D:578:LEU:HD12	2.00	0.43
1:A:373:VAL:O	1:A:548:PHE:HA	2.19	0.43
1:B:384:PHE:HA	1:B:387:LEU:HB2	2.00	0.43
1:C:584:LEU:HB2	1:D:578:LEU:HD21	1.99	0.43
1:D:15:PHE:CG	1:D:311:ILE:HG13	2.54	0.43
1:D:431:ILE:HD11	1:D:470:THR:OG1	2.19	0.43
1:A:578:LEU:O	1:A:582:ALA:HB2	2.19	0.43
1:D:384:PHE:HA	1:D:387:LEU:HB2	2.00	0.43
1:C:33:LEU:HD23	1:C:146:ILE:HD13	2.00	0.43
1:A:127:VAL:HG13	1:A:128:THR:HG23	2.01	0.43
1:B:457:ALA:HB1	1:B:461:ILE:HD13	2.00	0.43
1:C:18:LEU:HD11	1:C:321:LEU:HD13	2.01	0.43
1:A:547:LEU:HD22	1:A:554:ILE:HD13	2.00	0.42
1:B:440:GLU:O	1:B:440:GLU:CG	2.56	0.42
1:B:484:ARG:HA	1:B:487:ILE:HD12	2.01	0.42
1:B:547:LEU:HD22	1:B:554:ILE:HD13	2.01	0.42
1:B:15:PHE:O	1:B:19:VAL:HG23	2.18	0.42
1:C:486:ARG:HA	1:C:489:ILE:HD12	2.01	0.42
1:C:506:THR:CG2	1:C:514:GLU:HG2	2.48	0.42
1:D:225:GLU:HA	1:D:228:ARG:HG2	2.01	0.42
1:A:512:GLN:HE21	1:B:576:GLN:HB2	1.85	0.42
1:B:183:PRO:HA	1:B:186:ARG:HG2	2.01	0.42
1:B:197:ASP:O	1:B:201:ARG:HB2	2.19	0.42
1:C:346:VAL:HG13	1:C:393:PRO:HB3	2.01	0.42
1:A:197:ASP:OD2	1:A:316:ARG:NH2	2.52	0.42
1:D:405:VAL:HA	1:D:408:TYR:HD2	1.85	0.42
1:A:414:ARG:NH2	1:A:417:ILE:HG22	2.33	0.42
1:D:18:LEU:HD21	1:D:321:LEU:HD13	2.02	0.42
1:D:192:SER:O	1:D:196:GLN:HB2	2.19	0.42
1:D:443:VAL:HG11	1:D:494:LEU:HD11	2.00	0.42
1:B:202:PHE:N	1:B:202:PHE:HD1	2.18	0.42
1:A:207:ASN:O	1:A:211:PRO:HD3	2.19	0.42
1:C:563:LEU:HD21	1:C:570:TYR:CE2	2.54	0.42
1:D:206:LEU:C	1:D:206:LEU:CD1	2.85	0.42
1:A:537:LEU:H	1:A:577:GLN:NE2	2.17	0.42
1:B:138:ILE:HA	1:B:141:HIS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:LYS:O	1:D:241:VAL:HB	2.20	0.42
1:B:506:THR:HA	1:B:509:LEU:HB2	2.03	0.41
1:C:195:THR:HG23	1:C:196:GLN:HE22	1.73	0.41
1:D:484:ARG:HA	1:D:487:ILE:HD12	2.01	0.41
1:A:346:VAL:HG13	1:A:393:PRO:HB3	2.01	0.41
1:A:50:THR:HG22	1:A:53:LEU:HD13	2.03	0.41
1:A:138:ILE:HD12	1:A:141:HIS:ND1	2.35	0.41
1:D:18:LEU:HA	1:D:21:ARG:HG3	2.03	0.41
1:D:230:LYS:HD3	1:D:230:LYS:C	2.41	0.41
1:D:400:LEU:HD11	1:D:413:TRP:HE1	1.78	0.41
1:A:203:THR:HA	1:A:206:LEU:HG	2.01	0.41
1:A:389:ARG:HH22	1:A:406:ASP:HA	1.85	0.41
1:B:185:GLY:HA3	1:B:304:PHE:HE1	1.85	0.41
1:B:217:LYS:HA	1:B:221:ALA:CB	2.51	0.41
1:B:182:VAL:HG12	1:B:186:ARG:HE	1.86	0.41
1:B:456:TYR:O	1:B:456:TYR:CG	2.74	0.41
1:D:126:ARG:NH2	1:D:316:ARG:HH21	2.18	0.41
1:A:25:SER:OG	1:A:95:ILE:CD1	2.69	0.41
1:B:122:GLU:CG	1:B:201:ARG:HG3	2.51	0.41
1:C:145:PHE:O	1:C:149:ILE:HG12	2.21	0.41
1:A:484:ARG:HA	1:A:487:ILE:HD12	2.02	0.41
1:B:226:TYR:OH	1:B:230:LYS:HD3	2.21	0.41
1:C:484:ARG:HA	1:C:487:ILE:HD12	2.03	0.41
1:B:443:VAL:HG11	1:B:494:LEU:HD11	2.03	0.41
1:D:217:LYS:HZ2	1:D:221:ALA:HB3	1.86	0.40
1:D:332:LYS:HB3	1:D:334:ILE:HD12	2.02	0.40
1:A:104:TRP:CZ3	1:B:206:LEU:HD22	2.56	0.40
1:B:346:VAL:HG13	1:B:393:PRO:HB3	2.03	0.40
1:C:570:TYR:O	1:C:570:TYR:CG	2.72	0.40
1:D:217:LYS:HZ2	1:D:221:ALA:CB	2.34	0.40
1:D:567:HIS:CE1	1:D:570:TYR:HB2	2.56	0.40
1:A:68:GLY:HA2	1:A:72:LEU:HD13	2.03	0.40
1:A:166:LEU:HA	1:A:169:LEU:HD12	2.03	0.40
1:C:213:ILE:HA	1:C:216:VAL:HB	2.03	0.40
1:B:254:ILE:HD11	1:B:301:THR:HG21	2.04	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	567/599 (95%)	499 (88%)	64 (11%)	4 (1%)	22	60
1	B	565/599 (94%)	528 (94%)	33 (6%)	4 (1%)	22	60
1	C	561/599 (94%)	510 (91%)	49 (9%)	2 (0%)	34	70
1	D	568/599 (95%)	525 (92%)	38 (7%)	5 (1%)	17	54
All	All	2261/2396 (94%)	2062 (91%)	184 (8%)	15 (1%)	22	60

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404	PRO
1	A	428	SER
1	A	560	HIS
1	D	337	ALA
1	B	222	GLU
1	C	389	ARG
1	D	21	ARG
1	A	121	GLY
1	B	217	LYS
1	D	402	ASP
1	D	440	GLU
1	A	540	VAL
1	B	540	VAL
1	C	540	VAL
1	D	540	VAL

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	480/506 (95%)	456 (95%)	24 (5%)	24	52
1	B	481/506 (95%)	450 (94%)	31 (6%)	17	45
1	C	479/506 (95%)	453 (95%)	26 (5%)	22	50
1	D	480/506 (95%)	451 (94%)	29 (6%)	19	47
All	All	1920/2024 (95%)	1810 (94%)	110 (6%)	20	49

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	48	LEU
1	A	69	LEU
1	A	123	THR
1	A	142	ILE
1	A	146	ILE
1	A	156	LEU
1	A	169	LEU
1	A	186	ARG
1	A	196	GLN
1	A	233	ILE
1	A	258	LEU
1	A	288	LEU
1	A	294	ILE
1	A	311	ILE
1	A	372	ILE
1	A	383	LEU
1	A	413	TRP
1	A	440	GLU
1	A	445	ASP
1	A	477	ILE
1	A	518	GLN
1	A	537	LEU
1	A	562	GLU
1	B	21	ARG
1	B	41	LEU
1	B	48	LEU
1	B	67	ILE
1	B	95	ILE
1	B	123	THR
1	B	127	VAL

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Mol	Chain	Res	Type
1	B	142	ILE
1	B	146	ILE
1	B	156	LEU
1	B	169	LEU
1	B	191	ILE
1	B	254	ILE
1	B	258	LEU
1	B	288	LEU
1	B	289	TYR
1	B	294	ILE
1	B	311	ILE
1	B	330	THR
1	B	372	ILE
1	B	383	LEU
1	B	403	GLU
1	B	415	GLU
1	B	426	LEU
1	B	445	ASP
1	B	461	ILE
1	B	477	ILE
1	B	500	LEU
1	B	514	GLU
1	B	518	GLN
1	B	583	ASP
1	C	22	THR
1	C	48	LEU
1	C	66	GLN
1	C	95	ILE
1	C	127	VAL
1	C	131	THR
1	C	142	ILE
1	C	156	LEU
1	C	169	LEU
1	C	191	ILE
1	C	196	GLN
1	C	223	ASP
1	C	258	LEU
1	C	288	LEU
1	C	294	ILE
1	C	311	ILE
1	C	372	ILE
1	C	383	LEU

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Mol	Chain	Res	Type
1	C	407	THR
1	C	426	LEU
1	C	445	ASP
1	C	477	ILE
1	C	500	LEU
1	C	518	GLN
1	C	537	LEU
1	C	575	GLU
1	D	41	LEU
1	D	48	LEU
1	D	51	LYS
1	D	62	LEU
1	D	122	GLU
1	D	127	VAL
1	D	142	ILE
1	D	146	ILE
1	D	156	LEU
1	D	168	LEU
1	D	169	LEU
1	D	191	ILE
1	D	199	THR
1	D	234	SER
1	D	254	ILE
1	D	258	LEU
1	D	288	LEU
1	D	294	ILE
1	D	311	ILE
1	D	372	ILE
1	D	383	LEU
1	D	417	ILE
1	D	426	LEU
1	D	445	ASP
1	D	514	GLU
1	D	518	GLN
1	D	537	LEU
1	D	570	TYR
1	D	585	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN

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Mol	Chain	Res	Type
1	A	141	HIS
1	A	308	GLN
1	A	336	ASN
1	A	416	HIS
1	A	459	ASN
1	A	467	GLN
1	A	512	GLN
1	A	577	GLN
1	B	61	ASN
1	B	141	HIS
1	B	512	GLN
1	C	23	ASN
1	C	93	GLN
1	C	141	HIS
1	C	207	ASN
1	C	416	HIS
1	C	467	GLN
1	D	141	HIS
1	D	207	ASN
1	D	220	ASN
1	D	576	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	ATP	D	700	3	26,33,33	0.59	0	31,52,52	0.72	1 (3%)
2	ATP	A	700	3	26,33,33	0.62	0	31,52,52	0.76	1 (3%)
2	ATP	B	700	3	26,33,33	0.58	0	31,52,52	0.75	1 (3%)
2	ATP	C	700	3	26,33,33	0.57	0	31,52,52	0.72	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	700	3	-	2/18/38/38	0/3/3/3
2	ATP	A	700	3	-	5/18/38/38	0/3/3/3
2	ATP	B	700	3	-	2/18/38/38	0/3/3/3
2	ATP	C	700	3	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	ATP	C5-C6-N6	2.33	123.90	120.35
2	C	700	ATP	C5-C6-N6	2.29	123.84	120.35
2	D	700	ATP	C5-C6-N6	2.29	123.83	120.35
2	B	700	ATP	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	ATP	C5'-O5'-PA-O3A
2	A	700	ATP	PA-O3A-PB-O2B
2	A	700	ATP	PG-O3B-PB-O2B
2	B	700	ATP	PG-O3B-PB-O1B
2	D	700	ATP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	C	700	ATP	PG-O3B-PB-O1B
2	B	700	ATP	PB-O3B-PG-O2G
2	C	700	ATP	PB-O3B-PG-O2G
2	D	700	ATP	PB-O3B-PG-O2G
2	A	700	ATP	PG-O3B-PB-O1B
2	A	700	ATP	PA-O3A-PB-O1B

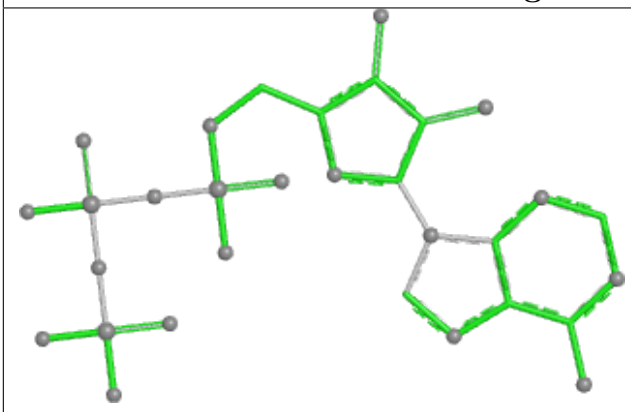
There are no ring outliers.

2 monomers are involved in 2 short contacts:

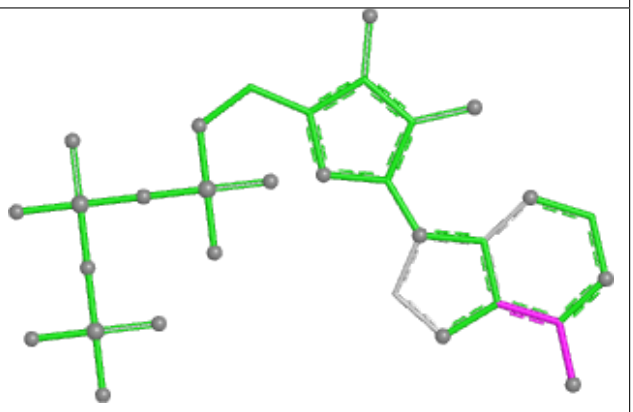
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	700	ATP	1	0
2	C	700	ATP	1	0

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.

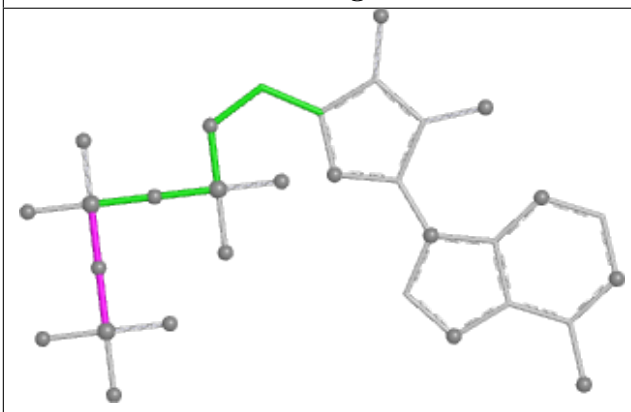
Ligand ATP D 700



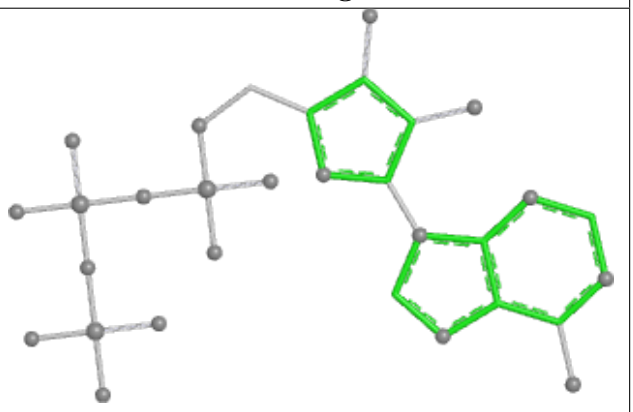
Bond lengths



Bond angles

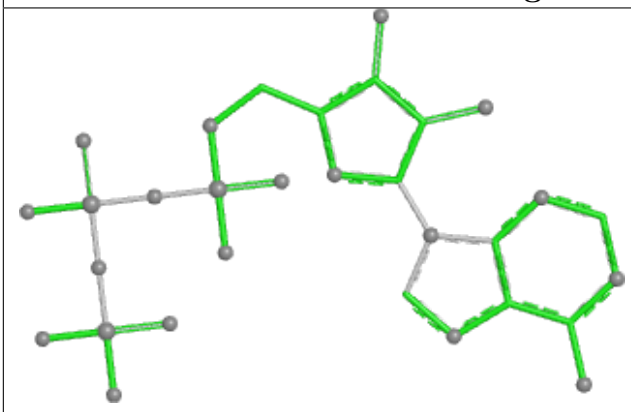


Torsions

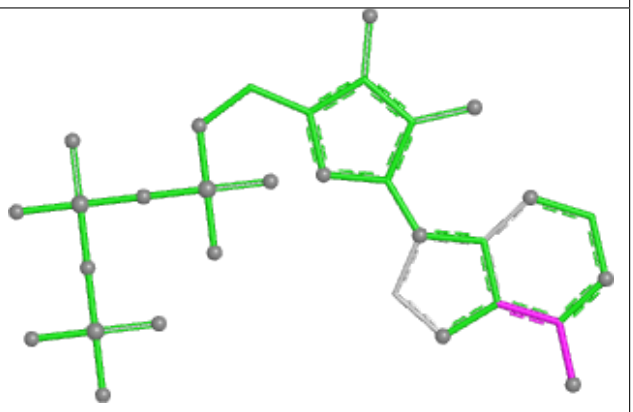


Rings

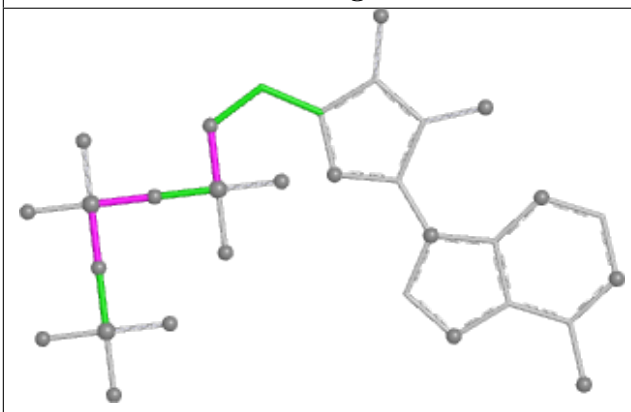
Ligand ATP A 700



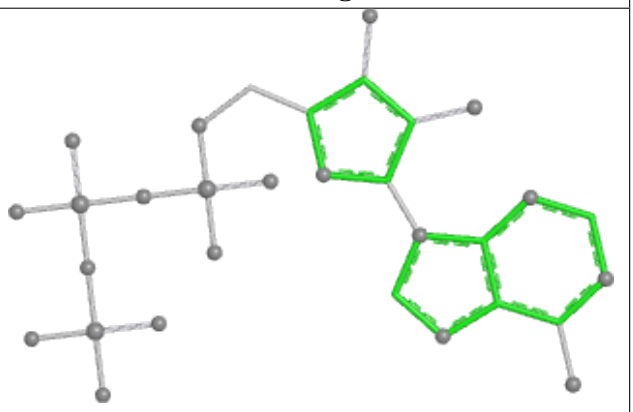
Bond lengths



Bond angles

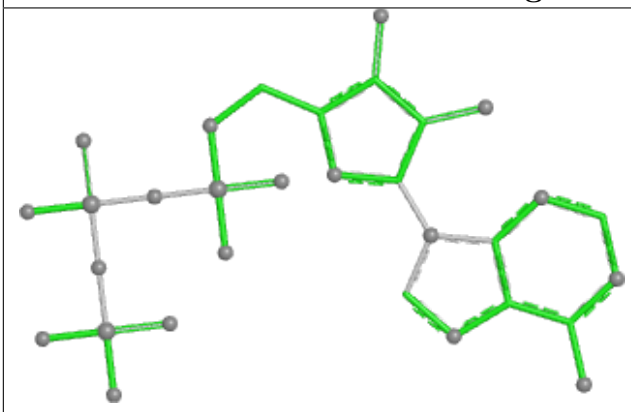


Torsions

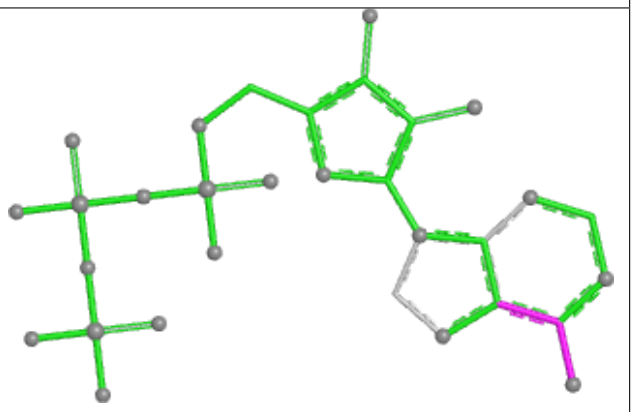


Rings

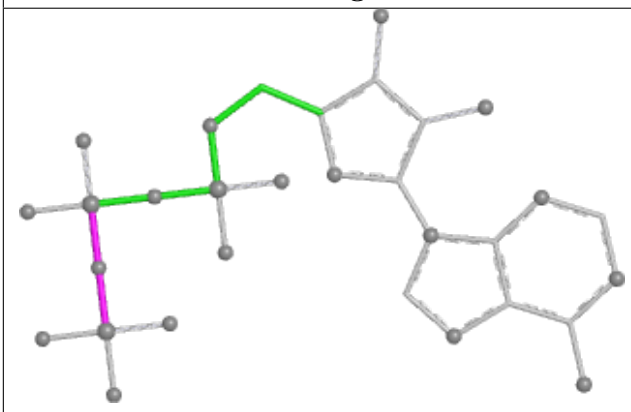
Ligand ATP B 700



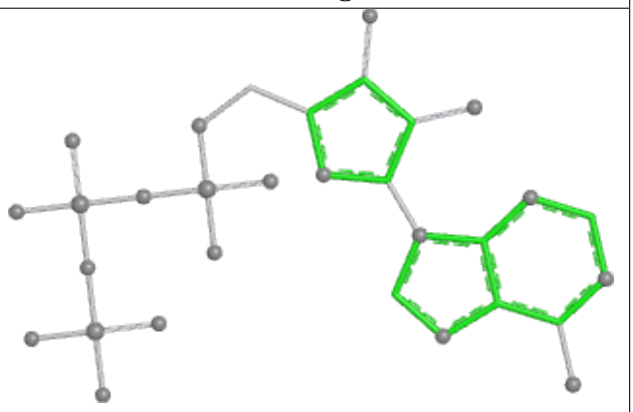
Bond lengths



Bond angles

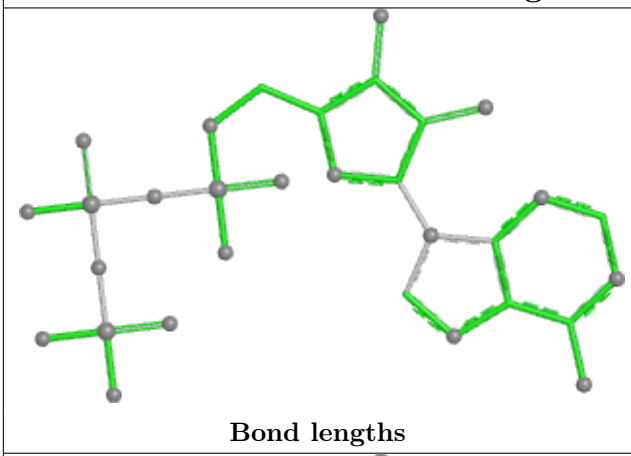


Torsions

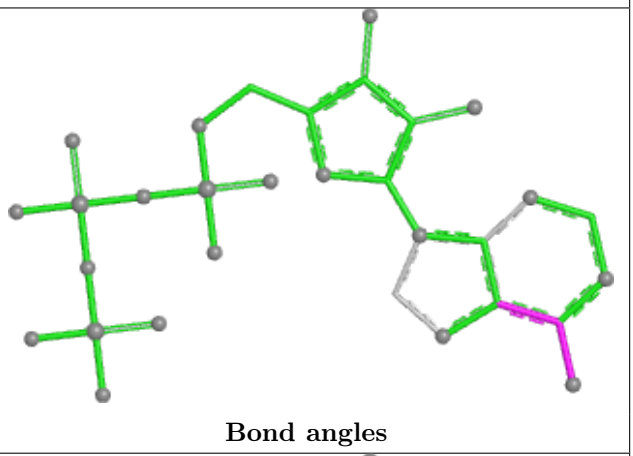


Rings

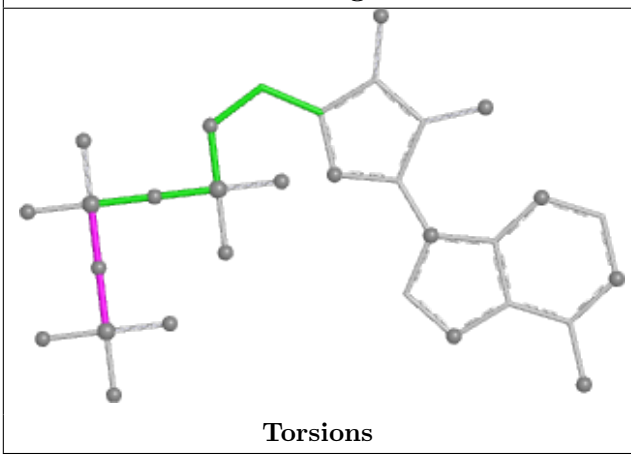
Ligand ATP C 700



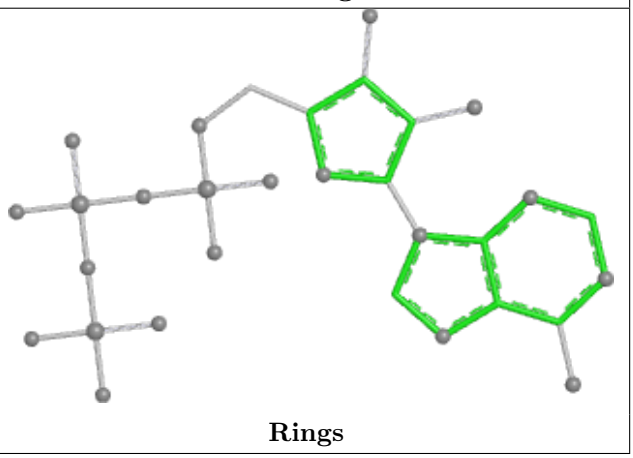
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	571/599 (95%)	0.13	39 (6%) 17 14	9, 75, 294, 300	0
1	B	569/599 (94%)	0.28	48 (8%) 11 10	18, 83, 295, 300	0
1	C	565/599 (94%)	0.20	51 (9%) 9 8	24, 75, 289, 300	0
1	D	572/599 (95%)	0.25	53 (9%) 8 8	21, 82, 300, 300	0
All	All	2277/2396 (95%)	0.21	191 (8%) 11 10	9, 79, 296, 300	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	572	ASP	13.8
1	B	336	ASN	10.2
1	A	395	ALA	10.1
1	C	55	ASP	9.7
1	A	329	VAL	9.5
1	D	589	GLY	8.2
1	D	588	ALA	8.0
1	A	441	ARG	7.5
1	D	68	GLY	7.2
1	D	442	ASP	7.0
1	A	440	GLU	6.8
1	A	336	ASN	6.6
1	D	394	THR	6.5
1	B	558	GLY	6.4
1	D	396	GLY	6.4
1	C	164	TRP	6.3
1	A	335	GLU	6.2
1	C	335	GLU	6.2
1	B	337	ALA	6.1
1	C	336	ASN	6.0
1	D	395	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	67	ILE	5.8
1	B	335	GLU	5.7
1	D	397	THR	5.6
1	A	397	THR	5.6
1	C	61	ASN	5.5
1	A	345	ARG	5.5
1	D	330	THR	5.4
1	D	345	ARG	5.4
1	B	58	SER	5.1
1	A	344	ASP	5.1
1	D	418	GLY	5.0
1	A	418	GLY	5.0
1	A	330	THR	5.0
1	C	333	GLN	4.9
1	A	396	GLY	4.9
1	A	279	THR	4.8
1	C	334	ILE	4.7
1	A	436	CYS	4.7
1	D	441	ARG	4.7
1	C	267	GLY	4.6
1	D	440	GLU	4.6
1	A	402	ASP	4.6
1	B	561	HIS	4.4
1	D	63	SER	4.4
1	D	439	LEU	4.4
1	B	331	GLY	4.4
1	A	442	ASP	4.3
1	B	358	LYS	4.3
1	C	54	VAL	4.2
1	D	571	ARG	4.2
1	C	544	ASP	4.1
1	C	58	SER	4.1
1	B	25	SER	4.1
1	D	402	ASP	4.1
1	D	565	ALA	4.0
1	D	568	GLY	3.9
1	D	219	SER	3.9
1	C	62	LEU	3.9
1	B	47	PRO	3.9
1	B	418	GLY	3.9
1	C	330	THR	3.9
1	D	587	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	57	PHE	3.8
1	B	534	ALA	3.8
1	B	533	ILE	3.8
1	D	70	ILE	3.8
1	C	402	ASP	3.8
1	A	218	ALA	3.7
1	B	26	TYR	3.7
1	A	566	SER	3.6
1	C	219	SER	3.6
1	D	64	GLY	3.6
1	B	580	MET	3.5
1	C	52	GLN	3.5
1	C	161	ILE	3.5
1	B	557	ARG	3.4
1	D	279	THR	3.4
1	A	565	ALA	3.4
1	B	455	ALA	3.4
1	D	573	PHE	3.4
1	B	353	ASP	3.3
1	A	568	GLY	3.3
1	B	441	ARG	3.3
1	D	570	TYR	3.3
1	B	347	SER	3.3
1	D	352	PRO	3.3
1	C	218	ALA	3.2
1	B	468	PHE	3.2
1	A	578	LEU	3.1
1	A	219	SER	3.1
1	B	285	ALA	3.0
1	C	568	GLY	3.0
1	A	331	GLY	2.9
1	D	359	GLU	2.9
1	B	222	GLU	2.9
1	D	328	THR	2.9
1	B	567	HIS	2.9
1	B	357	LEU	2.9
1	C	533	ILE	2.9
1	C	186	ARG	2.9
1	A	53	LEU	2.9
1	D	348	PHE	2.9
1	D	220	ASN	2.9
1	A	58	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	331	GLY	2.8
1	A	399	ARG	2.8
1	B	560	HIS	2.8
1	A	130	ASP	2.8
1	C	130	ASP	2.8
1	C	584	LEU	2.8
1	D	347	SER	2.8
1	B	354	GLN	2.8
1	B	284	VAL	2.8
1	C	65	THR	2.7
1	C	442	ASP	2.7
1	D	329	VAL	2.7
1	D	66	GLN	2.7
1	D	388	GLU	2.7
1	C	523	VAL	2.7
1	C	526	GLU	2.6
1	C	50	THR	2.6
1	B	584	LEU	2.6
1	C	63	SER	2.6
1	C	160	PHE	2.6
1	C	534	ALA	2.6
1	A	403	GLU	2.6
1	B	288	LEU	2.6
1	C	248	SER	2.6
1	D	13	LYS	2.6
1	C	268	TYR	2.6
1	A	342	GLN	2.5
1	C	407	THR	2.5
1	C	264	ALA	2.5
1	B	565	ALA	2.5
1	C	368	LYS	2.5
1	D	131	THR	2.5
1	B	52	GLN	2.5
1	A	55	ASP	2.5
1	B	48	LEU	2.4
1	B	49	LEU	2.4
1	C	283	LEU	2.4
1	B	247	GLN	2.4
1	A	328	THR	2.4
1	C	463	GLU	2.4
1	B	559	THR	2.4
1	A	45	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	469	ASP	2.4
1	D	280	ALA	2.4
1	C	53	LEU	2.3
1	B	50	THR	2.3
1	D	270	GLY	2.3
1	A	164	TRP	2.3
1	B	552	GLY	2.3
1	C	331	GLY	2.3
1	C	67	ILE	2.3
1	B	454	MET	2.3
1	A	443	VAL	2.3
1	D	61	ASN	2.3
1	D	293	ILE	2.3
1	A	332	LYS	2.3
1	C	51	LYS	2.3
1	C	57	PHE	2.3
1	C	403	GLU	2.3
1	D	349	GLY	2.2
1	D	574	ALA	2.2
1	B	544	ASP	2.2
1	D	344	ASP	2.2
1	B	91	ASN	2.2
1	B	188	MET	2.2
1	A	60	SER	2.2
1	D	292	GLN	2.2
1	C	56	GLY	2.2
1	D	218	ALA	2.1
1	C	64	GLY	2.1
1	B	377	GLY	2.1
1	B	332	LYS	2.1
1	C	418	GLY	2.1
1	B	453	GLU	2.1
1	A	269	GLY	2.1
1	D	469	ASP	2.1
1	B	62	LEU	2.1
1	C	265	VAL	2.1
1	B	355	LEU	2.1
1	C	374	GLY	2.1
1	D	421	SER	2.1
1	D	566	SER	2.0
1	C	388	GLU	2.0
1	D	69	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	47	PRO	2.0
1	A	61	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

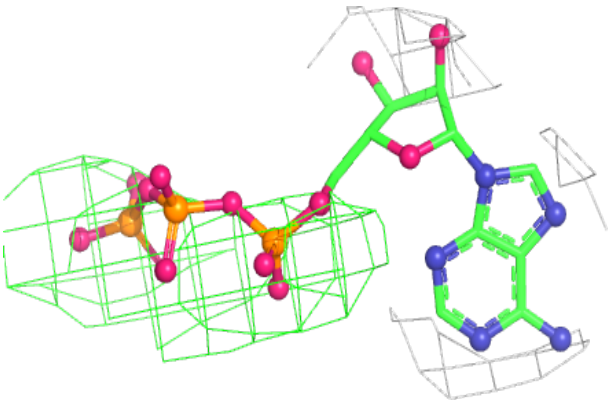
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

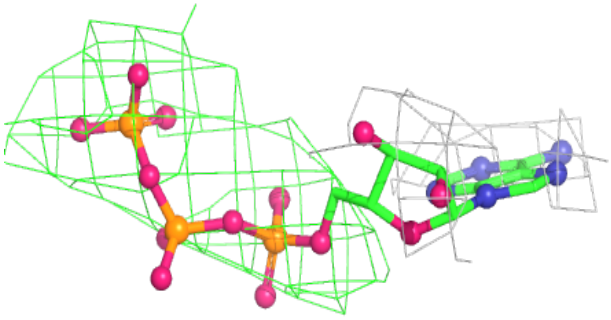
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ATP	D	700	31/31	0.87	0.32	43,55,65,70	0
2	ATP	B	700	31/31	0.90	0.31	39,54,62,63	0
2	ATP	C	700	31/31	0.94	0.20	30,37,43,48	0
2	ATP	A	700	31/31	0.94	0.19	33,41,49,50	0
3	MG	C	701	1/1	0.94	0.23	31,31,31,31	0
3	MG	D	701	1/1	0.94	0.36	41,41,41,41	0
3	MG	A	701	1/1	0.97	0.25	34,34,34,34	0
3	MG	B	701	1/1	0.97	0.34	43,43,43,43	0

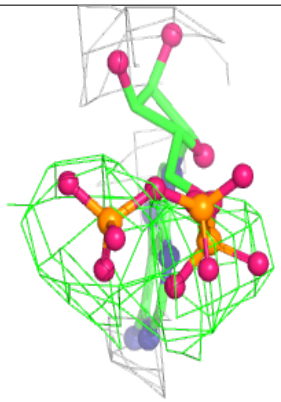
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP D 700:

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

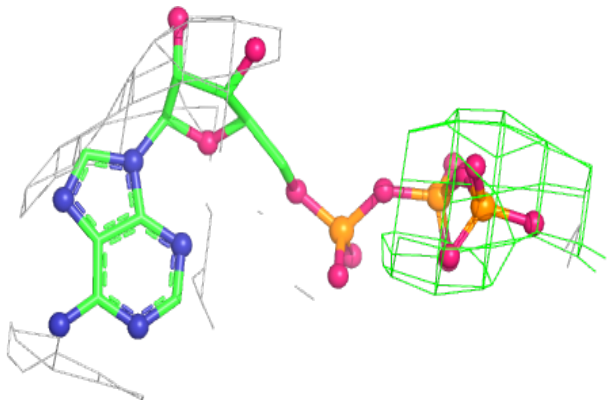


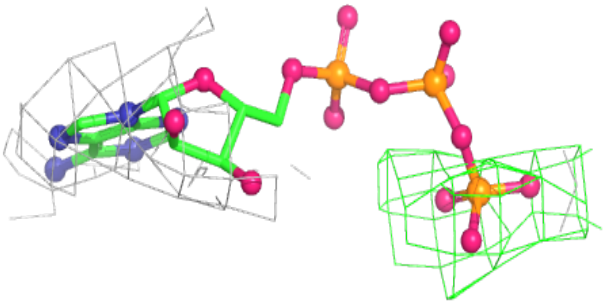


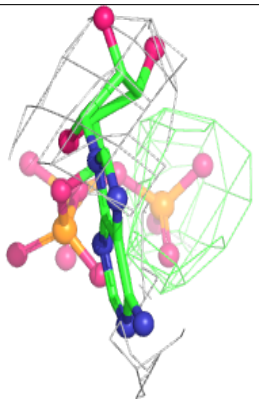


Electron density around ATP B 700:

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

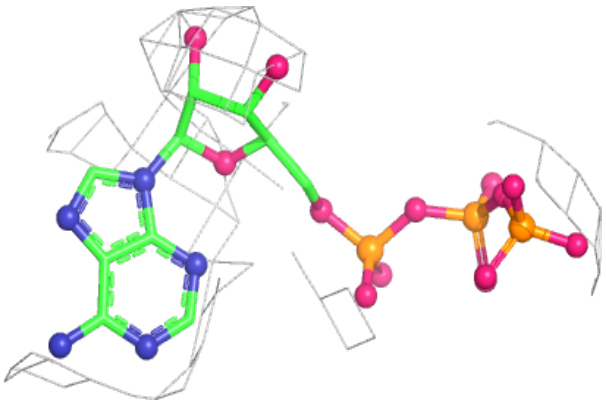


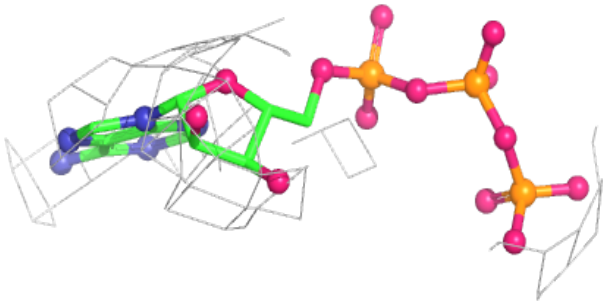


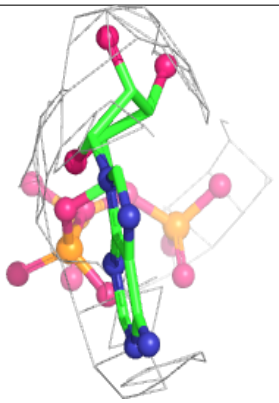


Electron density around ATP C 700:

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

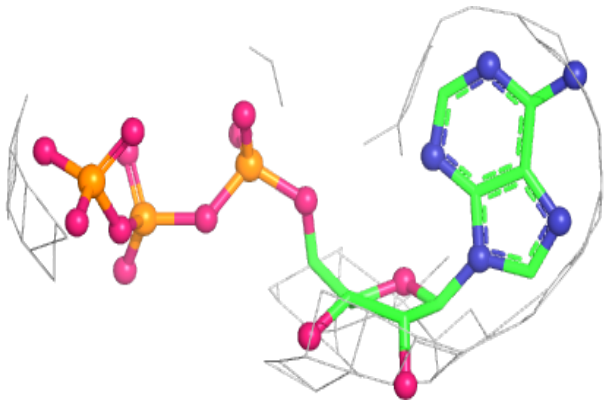


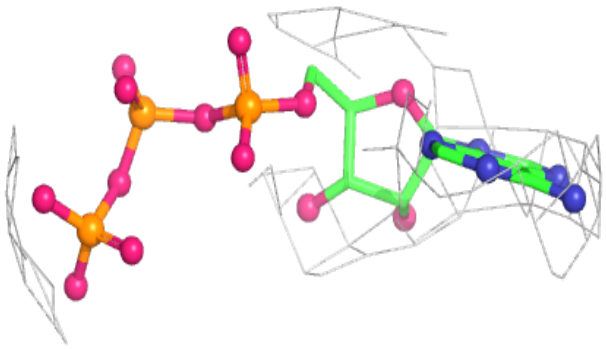


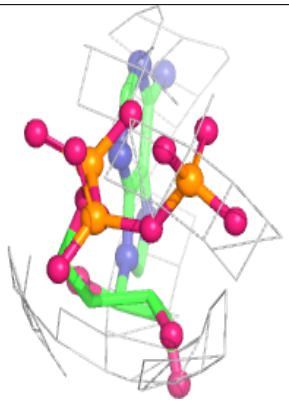


Electron density around ATP A 700:

$2mF_o$-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.