Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 11:54 pm GMT

PDB ID	:	6GFH
Title	:	Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from A. thaliana in complex with neo-IP5 and ATP
Authors	:	Whitfield, H.L.; Brearley, C.A.; Hemmings, A.M.
Deposited on	:	2018-04-30
Resolution	:	2.65 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:

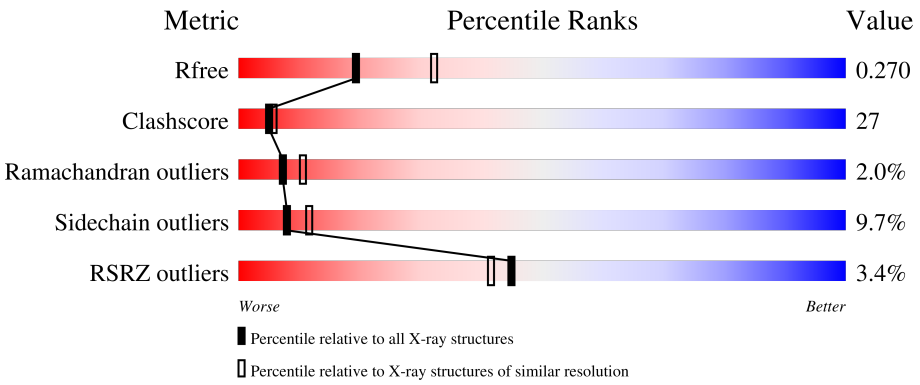
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	470	3% 52% 32% 5% 11%
1	B	470	3% 47% 34% 5% 13%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6970 atoms, of which 80 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 Inositol-pentakisphosphate 2-kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3341	2126	563	638	14	0	0	0
1	B	410	3275	2088	549	624	14	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A0A178UAB5
A	-17	ALA	-	expression tag	UNP A0A178UAB5
A	-16	HIS	-	expression tag	UNP A0A178UAB5
A	-15	HIS	-	expression tag	UNP A0A178UAB5
A	-14	HIS	-	expression tag	UNP A0A178UAB5
A	-13	HIS	-	expression tag	UNP A0A178UAB5
A	-12	HIS	-	expression tag	UNP A0A178UAB5
A	-11	HIS	-	expression tag	UNP A0A178UAB5
A	-10	SER	-	expression tag	UNP A0A178UAB5
A	-9	SER	-	expression tag	UNP A0A178UAB5
A	-8	GLY	-	expression tag	UNP A0A178UAB5
A	-7	LEU	-	expression tag	UNP A0A178UAB5
A	-6	GLU	-	expression tag	UNP A0A178UAB5
A	-5	VAL	-	expression tag	UNP A0A178UAB5
A	-4	LEU	-	expression tag	UNP A0A178UAB5
A	-3	PHE	-	expression tag	UNP A0A178UAB5
A	-2	GLN	-	expression tag	UNP A0A178UAB5
A	-1	GLY	-	expression tag	UNP A0A178UAB5
A	0	PRO	-	expression tag	UNP A0A178UAB5
A	185	MET	ILE	conflict	UNP A0A178UAB5
B	-18	MET	-	initiating methionine	UNP A0A178UAB5
B	-17	ALA	-	expression tag	UNP A0A178UAB5
B	-16	HIS	-	expression tag	UNP A0A178UAB5
B	-15	HIS	-	expression tag	UNP A0A178UAB5
B	-14	HIS	-	expression tag	UNP A0A178UAB5

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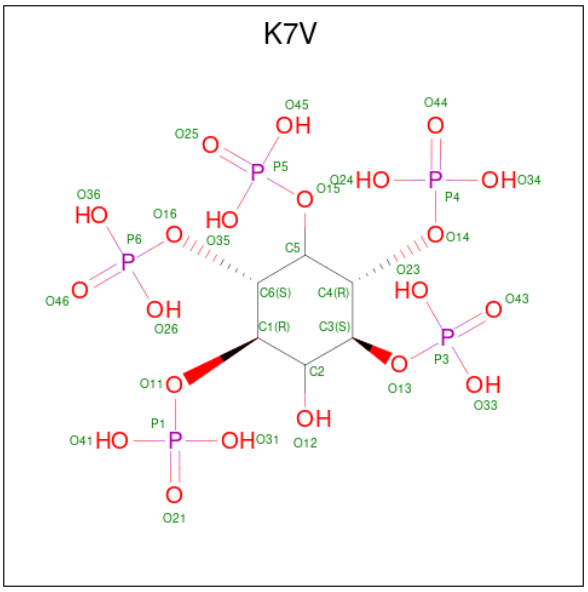
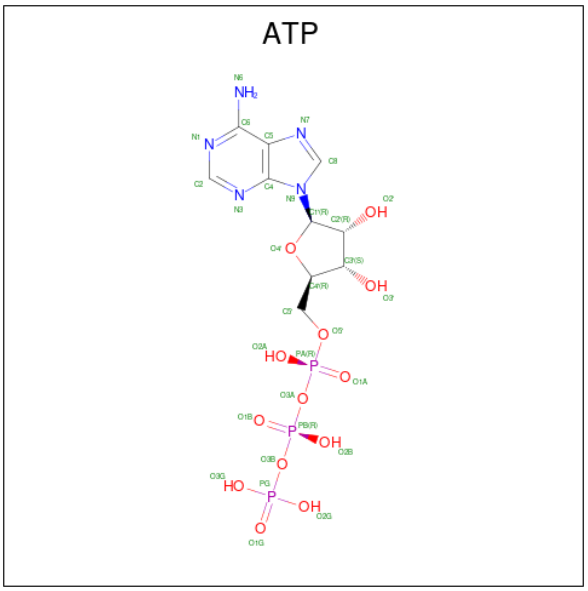
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP A0A178UAB5
B	-12	HIS	-	expression tag	UNP A0A178UAB5
B	-11	HIS	-	expression tag	UNP A0A178UAB5
B	-10	SER	-	expression tag	UNP A0A178UAB5
B	-9	SER	-	expression tag	UNP A0A178UAB5
B	-8	GLY	-	expression tag	UNP A0A178UAB5
B	-7	LEU	-	expression tag	UNP A0A178UAB5
B	-6	GLU	-	expression tag	UNP A0A178UAB5
B	-5	VAL	-	expression tag	UNP A0A178UAB5
B	-4	LEU	-	expression tag	UNP A0A178UAB5
B	-3	PHE	-	expression tag	UNP A0A178UAB5
B	-2	GLN	-	expression tag	UNP A0A178UAB5
B	-1	GLY	-	expression tag	UNP A0A178UAB5
B	0	PRO	-	expression tag	UNP A0A178UAB5
B	185	MET	ILE	conflict	UNP A0A178UAB5

- Molecule 2 is neo-Inositol pentakisphosphate (three-letter code: K7V) (formula: $C_6H_{17}O_{21}P_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			38	6	6	21	5		
2	B	1	Total	C	H	O	P	0	0
			38	6	6	21	5		

- Molecule 3 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	H	N	O	P		
3	A	1	43	10	12	5	13	3	0	0
3	B	1	43	10	12	5	13	3	0	0

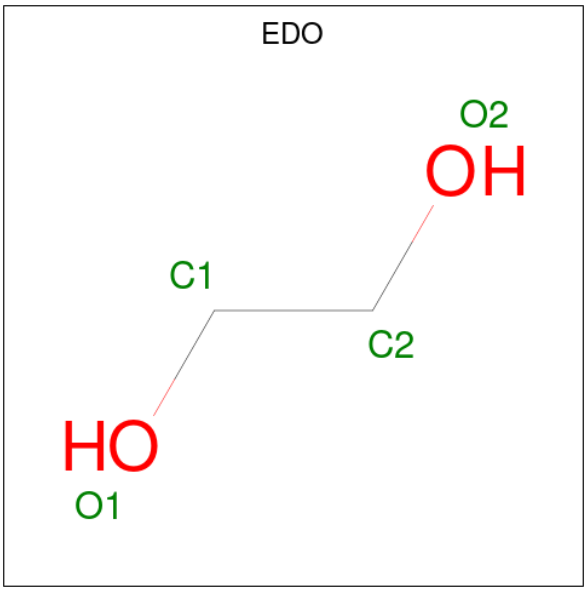
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	B	2	2	2	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

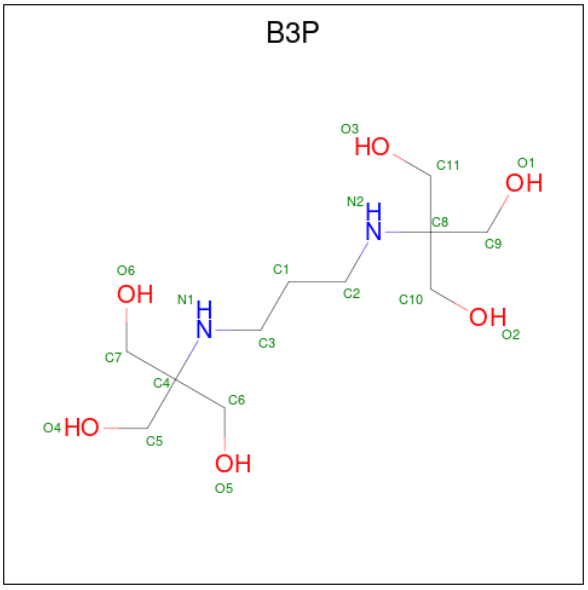
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0
5	B	1	1	1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	A	1	10	2	6	2	0	0
			Total	C	H	O		
6	A	1	10	2	6	2	0	0
			Total	C	H	O		
6	B	1	10	2	6	2	0	0

- Molecule 7 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	B	1	45	11	26	2	6	0	0

- Molecule 8 is water.

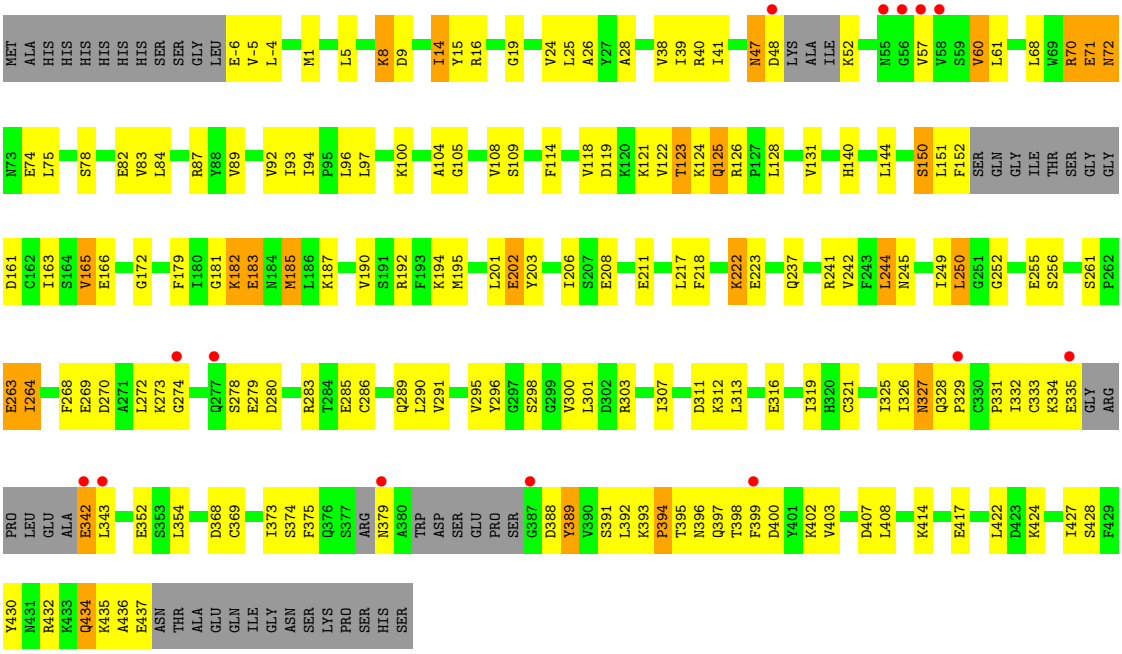
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	60	60	60	0	0
			Total	O		
8	B	52	52	52	0	0

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.

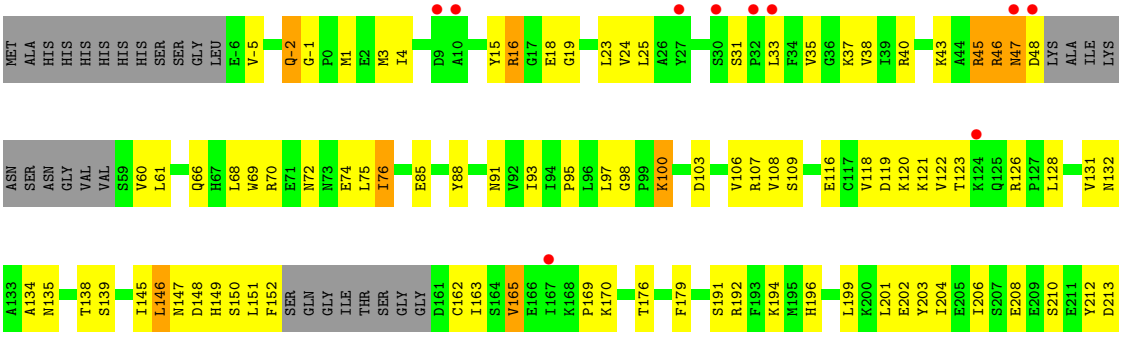
• Molecule 1: Inositol-pentakisphosphate 2-kinase

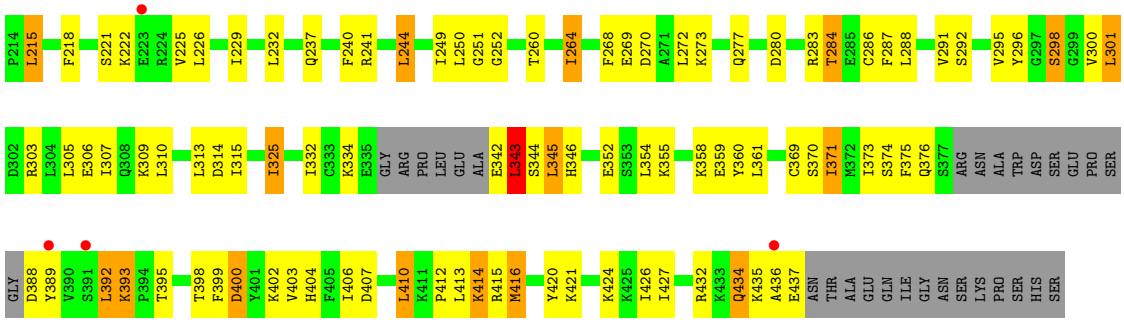
Chain A:



• Molecule 1: Inositol-pentakisphosphate 2-kinase

Chain B:




P214 L215 F218 S221 K222 E223 R224 V225 L226 I229 L232 Q237 F240 R241 L244 I249 L250 G251 G252 T260 I264 F268 E269 D270 A271 L272 K273 Q277 D280 R283 T284 E285 C286 F287 L288 V291 S292 V295 Y296 G297 S298 G299 V300 L301
D302 R303 L304 L305 E306 I307 Q308 K309 L310 L313 D314 I315 I325 I332 C333 K334 E335 GLY ARG PRO LEU GLU ALA E342 L343 S344 L345 H346 E352 S353 L354 K355 K358 E359 Y360 L361 C369 S370 I371 M372 I373 S374 F375 Q376 S377 ARG ASN ALA TRP ASP SER GLU PRO SER
GLY D388 Y389 V390 S391 L392 K393 P394 T395 T398 F399 D400 Y401 K402 V403 H404 F405 I406 D407 L410 K411 P412 L413 K414 R415 M416 Y420 K421 K424 K425 I426 I427 R432 K433 Q434 K435 A436 E437 ASN THR ALA GLU GLN ILE GLY ASN SER LYS PRO SER HIS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.63Å 60.56Å 84.48Å 87.81° 88.43° 63.01°	Depositor
Resolution (Å)	29.34 – 2.65 29.33 – 2.65	Depositor EDS
% Data completeness (in resolution range)	90.8 (29.34-2.65) 90.9 (29.33-2.65)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.199 , 0.268 0.201 , 0.270	Depositor DCC
R_{free} test set	1426 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l 0.017 for k,h,-l 0.012 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6970	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: K7V, ZN, ATP, EDO, MG, B3P

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	0.47	0/3399	0.58	0/4578
1	B	0.44	0/3334	0.59	1/4492 (0.0%)
All	All	0.46	0/6733	0.59	1/9070 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	410	LEU	CA-CB-CG	5.41	127.74	115.30

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	3341	0	3355	171	0
1	B	3275	0	3291	206	0
2	A	32	6	0	0	0
2	B	32	6	0	0	0
3	A	31	12	12	2	0
3	B	31	12	12	6	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	12	12	0	0
6	B	4	6	6	0	0
7	B	19	26	26	2	0
8	A	60	0	0	6	0
8	B	52	0	0	8	0
All	All	6890	80	6714	367	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 27.

All (367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:HA2	1:B:132:ASN:HD21	1.11	1.13
1:B:393:LYS:HE3	1:B:393:LYS:HA	1.40	1.03
1:B:74:GLU:HG3	1:B:91:ASN:ND2	1.81	0.94
1:B:74:GLU:HG3	1:B:91:ASN:HD22	1.31	0.94
1:A:261:SER:H	1:A:264:ILE:HD12	1.35	0.90
1:A:286:CYS:HB3	1:A:392:LEU:HD21	1.57	0.86
1:B:15:TYR:HB2	1:B:122:VAL:HB	1.60	0.84
1:B:301:LEU:HD11	1:B:371:ILE:HD11	1.61	0.82
1:B:260:THR:HG23	1:B:264:ILE:CG2	2.09	0.82
1:A:181:GLY:HA2	1:B:132:ASN:ND2	1.94	0.82
1:B:163:ILE:HD13	1:B:244:LEU:HA	1.64	0.79
1:B:18:GLU:OE1	1:B:126:ARG:NH1	2.16	0.79
1:B:18:GLU:OE2	1:B:126:ARG:HD2	1.83	0.79
1:B:4:ILE:HG12	1:B:109:SER:HB2	1.64	0.78
1:B:24:VAL:HG11	3:B:502:ATP:H5'1	1.65	0.78
1:A:74:GLU:HG2	1:A:87:ARG:HD3	1.66	0.78
1:B:342:GLU:HG2	1:B:345:LEU:HB2	1.67	0.76
1:B:392:LEU:HD23	1:B:395:THR:HG21	1.70	0.74
1:A:273:LYS:HA	1:A:283:ARG:NH1	2.01	0.74
1:A:303:ARG:O	1:A:307:ILE:HD12	1.87	0.74
1:A:72:ASN:HD22	1:A:75:LEU:H	1.35	0.73
1:A:252:GLY:HA3	1:A:255:GLU:O	1.88	0.73
1:B:97:LEU:HD13	1:B:307:ILE:CD1	2.19	0.73
1:B:210:SER:HB2	1:B:237:GLN:NE2	2.04	0.72
1:B:37:LYS:HE2	1:B:147:ASN:OD1	1.89	0.72
1:B:97:LEU:HD13	1:B:307:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LYS:HB2	1:B:414:LYS:NZ	2.03	0.72
1:A:60:VAL:HG22	1:A:61:LEU:HG	1.72	0.72
1:B:38:VAL:HG13	1:B:148:ASP:HB2	1.71	0.72
1:B:260:THR:HG23	1:B:264:ILE:HG22	1.73	0.71
1:B:40:ARG:NH1	3:B:502:ATP:O1A	2.24	0.71
1:B:334:LYS:HD3	8:B:621:HOH:O	1.91	0.71
1:B:74:GLU:CG	1:B:91:ASN:HD22	2.03	0.70
1:A:414:LYS:HE2	1:A:417:GLU:OE2	1.90	0.70
1:A:389:TYR:HB2	1:A:399:PHE:O	1.90	0.70
1:B:269:GLU:HG2	1:B:283:ARG:HH11	1.54	0.70
1:B:260:THR:HG23	1:B:264:ILE:HG21	1.73	0.70
1:B:272:LEU:HD12	1:B:284:THR:HG22	1.73	0.70
1:B:342:GLU:HG3	1:B:343:LEU:H	1.57	0.69
1:B:3:MET:CE	1:B:33:LEU:HD22	2.22	0.69
1:B:191:SER:HB3	1:B:215:LEU:HD21	1.73	0.69
1:B:424:LYS:HZ3	1:B:424:LYS:HB2	1.58	0.68
1:A:201:LEU:O	1:A:203:TYR:N	2.27	0.68
1:B:280:ASP:OD1	1:B:283:ARG:NH2	2.26	0.68
1:A:185:MET:HE1	8:A:643:HOH:O	1.92	0.68
1:A:244:LEU:HD12	1:A:245:ASN:N	2.09	0.68
1:A:179:PHE:HE2	1:A:313:LEU:HD22	1.59	0.67
1:A:104:ALA:HA	8:A:612:HOH:O	1.94	0.67
1:A:-6:GLU:HB3	8:A:640:HOH:O	1.95	0.67
1:A:182:LYS:HD3	1:B:132:ASN:ND2	2.09	0.67
1:A:187:LYS:HG3	1:A:427:ILE:HD13	1.77	0.67
1:B:3:MET:HE1	1:B:33:LEU:HD22	1.77	0.67
1:B:68:LEU:HD11	1:B:358:LYS:HG3	1.77	0.66
1:B:118:VAL:O	1:B:122:VAL:HG22	1.95	0.66
1:A:303:ARG:NH2	1:B:432:ARG:HH21	1.94	0.66
1:B:371:ILE:HG22	1:B:403:VAL:HG12	1.76	0.66
7:B:506:B3P:O5	7:B:506:B3P:O4	2.09	0.66
1:A:152:PHE:O	8:A:601:HOH:O	2.14	0.66
1:B:215:LEU:N	1:B:215:LEU:HD13	2.11	0.65
1:B:269:GLU:HG2	1:B:283:ARG:NH1	2.11	0.65
1:B:407:ASP:HB2	3:B:502:ATP:O2A	1.96	0.65
1:B:33:LEU:HD12	1:B:33:LEU:H	1.62	0.65
1:B:225:VAL:O	1:B:229:ILE:HD12	1.97	0.65
1:A:128:LEU:O	1:A:131:VAL:HG12	1.97	0.65
1:A:70:ARG:NH2	1:A:354:LEU:HD13	2.12	0.65
1:A:261:SER:N	1:A:264:ILE:HD12	2.08	0.64
1:B:199:LEU:HD23	1:B:426:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD13	1:A:307:ILE:HD13	1.80	0.64
1:B:16:ARG:NH2	1:B:148:ASP:OD2	2.30	0.64
1:A:222:LYS:HE2	1:A:296:TYR:CE2	2.32	0.63
1:A:89:VAL:O	1:A:94:ILE:HG13	1.99	0.63
1:B:342:GLU:HG3	1:B:344:SER:H	1.63	0.62
1:A:14:ILE:HD11	1:A:28:ALA:HB2	1.80	0.62
1:A:218:PHE:CE1	1:A:301:LEU:HD22	2.35	0.62
1:A:78:SER:HB3	1:A:83:VAL:HG13	1.81	0.62
1:A:182:LYS:HD3	1:A:182:LYS:H	1.65	0.61
1:A:312:LYS:NZ	1:B:202:GLU:HG3	2.14	0.61
1:A:179:PHE:CE2	1:A:313:LEU:HD22	2.36	0.61
1:B:301:LEU:HD11	1:B:371:ILE:CD1	2.30	0.61
1:A:93:ILE:HG21	1:A:408:LEU:HD13	1.82	0.61
1:A:201:LEU:C	1:A:203:TYR:H	2.02	0.61
1:A:333:CYS:SG	1:A:342:GLU:N	2.74	0.61
1:B:120:LYS:HE2	1:B:121:LYS:HZ3	1.65	0.61
1:B:192:ARG:HB3	8:B:640:HOH:O	2.01	0.60
1:B:16:ARG:HB3	1:B:24:VAL:O	2.00	0.60
1:B:151:LEU:HG	1:B:152:PHE:N	2.16	0.60
1:B:229:ILE:HG22	1:B:288:LEU:HB3	1.84	0.60
1:B:45:ARG:HB3	1:B:45:ARG:HH11	1.66	0.60
1:A:249:ILE:O	1:A:249:ILE:HG13	2.02	0.60
1:A:373:ILE:HD12	1:A:373:ILE:H	1.67	0.60
1:A:5:LEU:HD11	1:A:108:VAL:HG21	1.82	0.59
1:A:182:LYS:HD2	1:B:132:ASN:HA	1.84	0.59
1:B:74:GLU:OE1	1:B:74:GLU:N	2.29	0.59
1:B:152:PHE:HB3	1:B:376:GLN:NE2	2.17	0.59
1:A:222:LYS:HE2	1:A:296:TYR:CD2	2.37	0.59
1:B:270:ASP:O	1:B:273:LYS:HG2	2.03	0.59
1:A:150:SER:O	1:A:151:LEU:HD23	2.03	0.59
1:A:72:ASN:HD21	1:A:74:GLU:HB3	1.68	0.59
1:B:24:VAL:C	1:B:25:LEU:HD23	2.22	0.59
1:A:395:THR:O	1:A:397:GLN:N	2.32	0.59
1:B:287:PHE:CD2	1:B:288:LEU:HD23	2.38	0.59
1:A:5:LEU:HD12	1:A:5:LEU:N	2.18	0.58
1:B:414:LYS:HB2	1:B:414:LYS:HZ2	1.64	0.58
1:A:82:GLU:OE2	1:A:140:HIS:ND1	2.31	0.58
1:B:389:TYR:HA	1:B:399:PHE:O	2.03	0.58
1:A:5:LEU:HD12	1:A:5:LEU:H	1.67	0.58
1:A:374:SER:OG	1:A:402:LYS:HG3	2.04	0.58
1:B:241:ARG:HG2	1:B:251:GLY:HA3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:HG2	1:B:75:LEU:N	2.18	0.57
1:A:60:VAL:HG11	1:A:78:SER:O	2.04	0.57
1:A:222:LYS:HG2	1:A:223:GLU:OE1	2.04	0.57
1:B:325:ILE:HG13	1:B:354:LEU:HD23	1.85	0.57
1:A:181:GLY:CA	1:B:132:ASN:HD21	2.01	0.57
1:A:195:MET:CE	1:A:427:ILE:HD12	2.35	0.57
1:B:221:SER:O	1:B:225:VAL:HG23	2.06	0.56
1:B:-2:GLN:HE21	1:B:-1:GLY:H	1.54	0.56
1:A:278:SER:HB3	1:A:283:ARG:HG2	1.87	0.56
1:A:192:ARG:HH22	1:A:422:LEU:HD23	1.71	0.56
1:A:222:LYS:HB3	1:A:296:TYR:CD2	2.41	0.56
1:B:305:LEU:O	1:B:309:LYS:HG3	2.06	0.56
1:A:47:ASN:O	1:A:48:ASP:HB2	2.06	0.55
1:B:106:VAL:HG13	1:B:145:ILE:HB	1.88	0.55
1:A:122:VAL:O	1:A:124:LYS:N	2.39	0.55
1:A:97:LEU:HD13	1:A:307:ILE:CD1	2.36	0.55
1:A:190:VAL:HG12	1:A:194:LYS:HB3	1.87	0.55
1:B:116:GLU:HG3	1:B:138:THR:CG2	2.36	0.55
1:A:270:ASP:O	1:A:273:LYS:HG2	2.07	0.55
1:A:279:GLU:H	1:A:279:GLU:CD	2.10	0.55
1:A:343:LEU:HD13	1:A:343:LEU:O	2.07	0.55
1:A:195:MET:HE3	1:A:427:ILE:HD12	1.89	0.55
1:B:201:LEU:HD23	1:B:206:ILE:HG13	1.88	0.55
1:B:392:LEU:HD23	1:B:395:THR:CG2	2.36	0.55
1:A:237:GLN:HA	1:A:256:SER:HB2	1.90	0.54
1:B:66:GLN:O	1:B:76:ILE:HD11	2.07	0.54
1:B:412:PRO:O	1:B:415:ARG:HB3	2.08	0.54
1:A:119:ASP:O	1:A:123:THR:HG23	2.07	0.54
1:B:226:LEU:HD13	1:B:292:SER:CB	2.38	0.54
1:B:204:ILE:O	1:B:204:ILE:HG22	2.07	0.54
1:B:15:TYR:HB2	1:B:122:VAL:CB	2.35	0.54
1:A:192:ARG:NH2	1:A:422:LEU:HD23	2.23	0.54
1:A:24:VAL:O	1:A:25:LEU:HD23	2.07	0.54
1:A:392:LEU:HD23	1:A:395:THR:OG1	2.07	0.54
1:B:149:HIS:O	1:B:374:SER:HB3	2.07	0.54
1:A:379:ASN:OD1	1:A:398:THR:HG22	2.08	0.53
1:B:414:LYS:HE3	8:B:636:HOH:O	2.06	0.53
1:A:223:GLU:OE1	1:A:223:GLU:N	2.39	0.53
1:A:298:SER:CB	1:A:300:VAL:HG13	2.38	0.53
1:B:152:PHE:CD2	1:B:376:GLN:HB2	2.42	0.53
1:B:373:ILE:HG23	1:B:403:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:HG13	1:A:242:VAL:HG22	1.89	0.53
1:A:187:LYS:NZ	1:A:316:GLU:HG3	2.24	0.53
1:B:106:VAL:CG1	1:B:145:ILE:HB	2.38	0.53
1:A:298:SER:OG	1:A:300:VAL:HG13	2.08	0.53
1:A:237:GLN:CA	1:A:256:SER:HB2	2.40	0.53
1:A:8:LYS:HD2	1:A:9:ASP:CG	2.30	0.52
1:A:291:VAL:O	1:A:295:VAL:HG23	2.09	0.52
1:B:68:LEU:CD1	1:B:358:LYS:HG3	2.39	0.52
1:B:163:ILE:O	1:B:375:PHE:HB2	2.09	0.52
1:A:5:LEU:CD1	1:A:108:VAL:HG21	2.39	0.52
1:B:373:ILE:HG12	1:B:403:VAL:HG13	1.92	0.52
1:B:163:ILE:HD11	1:B:244:LEU:HG	1.90	0.52
1:B:269:GLU:CG	1:B:283:ARG:HH11	2.21	0.52
1:A:303:ARG:HH22	1:B:432:ARG:HH21	1.57	0.52
1:B:19:GLY:O	1:B:43:LYS:NZ	2.34	0.52
1:B:126:ARG:NH2	1:B:134:ALA:O	2.42	0.52
1:B:148:ASP:OD1	1:B:150:SER:OG	2.26	0.52
1:A:274:GLY:H	1:A:283:ARG:NH1	2.08	0.52
1:B:126:ARG:NH2	1:B:131:VAL:HA	2.24	0.52
1:B:229:ILE:HD13	1:B:292:SER:HA	1.92	0.52
1:A:237:GLN:C	1:A:256:SER:HB2	2.30	0.52
1:B:269:GLU:CD	1:B:284:THR:HG23	2.30	0.52
1:B:392:LEU:HG	1:B:395:THR:HG22	1.91	0.52
1:A:126:ARG:NH1	1:A:131:VAL:HG23	2.25	0.51
1:A:201:LEU:C	1:A:203:TYR:N	2.63	0.51
1:B:407:ASP:OD2	3:B:502:ATP:O2B	2.28	0.51
1:A:342:GLU:O	1:A:343:LEU:HB3	2.09	0.51
1:A:-5:VAL:HG12	8:A:640:HOH:O	2.09	0.51
1:A:393:LYS:HB3	1:A:394:PRO:HD3	1.91	0.51
1:A:26:ALA:HA	1:A:38:VAL:HG12	1.91	0.51
1:A:39:ILE:HA	1:A:144:LEU:O	2.11	0.51
1:A:39:ILE:HG12	1:A:41:ILE:HD11	1.93	0.51
1:A:329:PRO:O	1:A:331:PRO:HD3	2.11	0.51
1:B:116:GLU:HG3	1:B:138:THR:HG21	1.92	0.51
1:B:74:GLU:HG2	1:B:75:LEU:H	1.75	0.51
1:B:97:LEU:HD13	1:B:307:ILE:HD12	1.91	0.51
1:A:182:LYS:H	1:A:182:LYS:CD	2.22	0.51
1:B:151:LEU:HD12	1:B:152:PHE:H	1.75	0.51
1:A:118:VAL:O	1:A:122:VAL:HG13	2.12	0.50
1:A:72:ASN:ND2	1:A:75:LEU:H	2.06	0.50
1:B:212:TYR:HB2	1:B:232:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:O	1:B:100:LYS:NZ	2.41	0.50
1:A:182:LYS:NZ	1:B:132:ASN:HB2	2.27	0.50
1:A:312:LYS:HZ3	1:B:202:GLU:HG3	1.77	0.50
1:A:373:ILE:HG23	1:A:403:VAL:HG22	1.92	0.50
1:B:191:SER:HB3	1:B:215:LEU:CD2	2.42	0.50
1:B:393:LYS:HA	1:B:393:LYS:CE	2.26	0.49
1:A:298:SER:HB2	1:A:300:VAL:HG13	1.94	0.49
1:A:163:ILE:O	1:A:375:PHE:HB2	2.13	0.49
1:B:229:ILE:CG2	1:B:288:LEU:HB3	2.41	0.49
1:B:95:PRO:HB2	8:B:638:HOH:O	2.12	0.49
1:A:290:LEU:HD21	1:A:399:PHE:CD1	2.47	0.49
1:B:260:THR:CG2	1:B:264:ILE:HG22	2.41	0.49
1:A:105:GLY:HA3	1:A:144:LEU:HD22	1.95	0.48
1:B:45:ARG:O	1:B:47:ASN:N	2.46	0.48
1:B:69:TRP:C	1:B:76:ILE:HD12	2.33	0.48
1:A:222:LYS:HB3	1:A:296:TYR:CE2	2.48	0.48
1:A:211:GLU:HA	1:A:211:GLU:OE1	2.13	0.48
1:B:119:ASP:OD1	1:B:135:ASN:ND2	2.47	0.48
1:A:163:ILE:HD13	1:A:244:LEU:HA	1.95	0.48
1:B:148:ASP:OD1	1:B:150:SER:N	2.47	0.48
1:A:121:LYS:HE3	1:A:125:GLN:HE22	1.79	0.48
1:B:-2:GLN:OE1	1:B:1:MET:HG3	2.14	0.47
1:B:45:ARG:C	1:B:47:ASN:H	2.17	0.47
1:B:300:VAL:HG21	1:B:403:VAL:HG11	1.96	0.47
1:B:213:ASP:OD1	1:B:215:LEU:HD22	2.14	0.47
1:B:306:GLU:OE1	1:B:306:GLU:HA	2.14	0.47
1:A:398:THR:HG23	1:A:398:THR:O	2.14	0.47
1:A:273:LYS:HG3	1:A:273:LYS:O	2.13	0.47
1:A:335:GLU:O	1:A:335:GLU:HG2	2.14	0.47
1:B:301:LEU:HD12	1:B:301:LEU:HA	1.66	0.47
1:B:421:LYS:HD3	8:B:642:HOH:O	2.15	0.47
1:A:202:GLU:O	1:A:202:GLU:HG3	2.15	0.47
1:A:333:CYS:O	1:A:334:LYS:HG2	2.13	0.47
1:B:47:ASN:O	1:B:48:ASP:CB	2.62	0.47
1:B:283:ARG:O	1:B:286:CYS:HB2	2.14	0.47
1:B:303:ARG:O	1:B:307:ILE:HG13	2.15	0.47
1:B:315:ILE:CD1	1:B:416:MET:CE	2.92	0.47
1:A:249:ILE:O	1:A:250:LEU:HB2	2.15	0.47
1:B:88:TYR:CE1	1:B:410:LEU:HD13	2.50	0.47
1:B:47:ASN:N	1:B:47:ASN:OD1	2.47	0.47
1:B:169:PRO:O	1:B:170:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:TYR:CG	1:B:232:LEU:HD21	2.50	0.46
1:B:240:PHE:HE1	1:B:250:LEU:HD23	1.80	0.46
1:B:376:GLN:HB3	1:B:400:ASP:OD1	2.16	0.46
1:B:18:GLU:CD	1:B:126:ARG:HD2	2.35	0.46
1:B:407:ASP:CG	3:B:502:ATP:O2G	2.53	0.46
1:B:108:VAL:HG22	1:B:109:SER:N	2.29	0.46
1:B:108:VAL:HG22	1:B:109:SER:O	2.15	0.46
1:A:398:THR:O	1:A:398:THR:CG2	2.62	0.46
1:B:315:ILE:HD13	1:B:416:MET:CE	2.46	0.46
1:B:46:ARG:HG3	1:B:46:ARG:HH11	1.81	0.46
1:B:199:LEU:O	1:B:203:TYR:HD2	1.98	0.46
1:B:310:LEU:HB3	1:B:359:GLU:HB3	1.98	0.46
1:A:244:LEU:O	1:A:245:ASN:C	2.54	0.46
1:A:289:GLN:O	1:A:289:GLN:HG3	2.15	0.46
1:A:326:ILE:O	1:A:327:ASN:O	2.34	0.46
1:A:428:SER:O	1:A:432:ARG:HG3	2.16	0.46
1:B:345:LEU:HA	1:B:345:LEU:HD12	1.60	0.45
1:B:24:VAL:HG11	3:B:502:ATP:C5'	2.43	0.45
1:B:98:GLY:N	8:B:602:HOH:O	2.48	0.45
1:A:244:LEU:HD12	1:A:245:ASN:H	1.82	0.45
1:B:151:LEU:CG	1:B:152:PHE:N	2.80	0.45
1:B:222:LYS:HG3	1:B:296:TYR:CG	2.51	0.45
1:B:298:SER:OG	1:B:300:VAL:HG22	2.16	0.45
1:A:343:LEU:O	1:A:343:LEU:HD22	2.16	0.45
1:A:206:ILE:HB	8:A:626:HOH:O	2.15	0.45
1:A:434:GLN:O	1:A:437:GLU:HG3	2.16	0.45
1:B:45:ARG:HB3	1:B:45:ARG:NH1	2.31	0.45
1:B:212:TYR:CD1	1:B:232:LEU:HD21	2.51	0.45
1:B:60:VAL:O	1:B:61:LEU:HD23	2.17	0.45
1:B:165:VAL:HG11	1:B:291:VAL:HG22	1.98	0.45
1:B:240:PHE:CE1	1:B:250:LEU:HD23	2.52	0.45
1:B:97:LEU:CD1	1:B:307:ILE:HD11	2.45	0.45
1:A:179:PHE:HE2	1:A:313:LEU:CD2	2.28	0.44
1:B:31:SER:O	1:B:35:VAL:HG23	2.17	0.44
1:B:334:LYS:HB3	8:B:616:HOH:O	2.16	0.44
1:B:38:VAL:HG22	1:B:146:LEU:O	2.17	0.44
1:A:183:GLU:CD	1:A:183:GLU:H	2.20	0.44
1:A:195:MET:HE3	1:A:430:TYR:HB3	1.99	0.44
1:B:287:PHE:HD2	1:B:288:LEU:HD23	1.81	0.44
1:B:434:GLN:C	1:B:436:ALA:H	2.21	0.44
1:A:182:LYS:HD3	1:A:182:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:HG3	1:B:46:ARG:NH1	2.32	0.44
1:B:342:GLU:O	1:B:343:LEU:HB2	2.17	0.44
1:B:74:GLU:CG	1:B:75:LEU:N	2.80	0.44
1:A:182:LYS:HZ3	1:B:132:ASN:HD22	1.65	0.44
1:A:39:ILE:HG12	1:A:41:ILE:CD1	2.48	0.44
1:A:424:LYS:O	1:A:428:SER:HB2	2.18	0.44
1:B:15:TYR:HB2	1:B:122:VAL:CG1	2.48	0.44
1:B:25:LEU:HD23	1:B:25:LEU:N	2.32	0.44
1:B:46:ARG:HH21	1:B:135:ASN:HB2	1.83	0.43
1:B:369:CYS:HB2	1:B:406:ILE:O	2.19	0.43
1:B:414:LYS:NZ	1:B:414:LYS:CB	2.74	0.43
1:A:279:GLU:OE1	1:A:279:GLU:N	2.50	0.43
1:B:334:LYS:HA	8:B:621:HOH:O	2.17	0.43
1:A:100:LYS:O	1:A:100:LYS:HG2	2.18	0.43
1:B:414:LYS:HB2	1:B:414:LYS:HZ3	1.80	0.43
1:A:269:GLU:OE2	1:A:283:ARG:HG3	2.19	0.43
1:B:68:LEU:HD22	1:B:413:LEU:HD13	1.99	0.43
1:A:92:VAL:O	1:A:96:LEU:HD12	2.19	0.43
1:A:393:LYS:CB	1:A:394:PRO:HD3	2.48	0.43
1:B:303:ARG:HD2	1:B:303:ARG:HA	1.68	0.43
1:A:172:GLY:HA3	1:A:218:PHE:CD2	2.53	0.43
1:A:52:LYS:HA	1:A:57:VAL:O	2.18	0.43
1:A:325:ILE:HD12	1:A:354:LEU:CD2	2.49	0.43
1:A:-4:LEU:HD12	1:A:-4:LEU:HA	1.67	0.43
1:B:-2:GLN:NE2	1:B:-1:GLY:H	2.16	0.43
1:B:38:VAL:HG13	1:B:148:ASP:CB	2.44	0.43
1:B:301:LEU:CD1	1:B:371:ILE:CD1	2.97	0.43
1:A:60:VAL:HG23	1:A:84:LEU:HD22	2.01	0.43
1:B:424:LYS:HB2	1:B:424:LYS:NZ	2.26	0.43
1:B:392:LEU:CG	1:B:395:THR:HG22	2.49	0.42
1:A:5:LEU:HB3	1:A:114:PHE:CD2	2.53	0.42
1:A:379:ASN:HD21	1:A:398:THR:H	1.66	0.42
1:B:74:GLU:CG	1:B:75:LEU:H	2.31	0.42
1:A:41:ILE:HD12	1:A:41:ILE:N	2.34	0.42
1:A:436:ALA:O	1:A:437:GLU:HB3	2.18	0.42
1:B:332:ILE:HD12	1:B:420:TYR:CZ	2.54	0.42
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.87	0.42
1:B:40:ARG:HH11	1:B:40:ARG:HD2	1.70	0.42
1:A:121:LYS:HD2	1:A:121:LYS:O	2.19	0.42
1:A:268:PHE:CE2	1:A:272:LEU:HD11	2.55	0.42
1:B:346:HIS:HB3	7:B:506:B3P:H12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ASP:HB2	1:B:402:LYS:NZ	2.35	0.42
1:A:194:LYS:HB2	1:A:194:LYS:HE3	1.79	0.42
1:A:217:LEU:HG	1:A:301:LEU:CD1	2.50	0.42
1:B:23:LEU:HG	1:B:25:LEU:HD21	2.01	0.42
1:B:427:ILE:HD12	1:B:427:ILE:HA	1.77	0.42
1:B:434:GLN:HG3	1:B:435:LYS:N	2.34	0.42
1:B:163:ILE:HD13	1:B:163:ILE:HA	1.89	0.42
1:B:170:LYS:HD2	1:B:170:LYS:HA	1.75	0.42
1:B:315:ILE:HB	1:B:360:TYR:OH	2.20	0.42
1:B:325:ILE:HD12	1:B:325:ILE:HA	1.79	0.42
1:A:195:MET:CE	1:A:427:ILE:HA	2.50	0.41
1:A:222:LYS:HB2	1:A:222:LYS:HZ3	1.85	0.41
1:B:313:LEU:O	1:B:314:ASP:HB3	2.19	0.41
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.93	0.41
1:A:369:CYS:HB3	1:A:408:LEU:HD23	2.01	0.41
1:B:149:HIS:CD2	1:B:404:HIS:CG	3.08	0.41
1:B:268:PHE:HZ	1:B:287:PHE:CE2	2.38	0.41
1:B:334:LYS:HD3	1:B:334:LYS:HA	1.91	0.41
1:A:166:GLU:OE1	1:A:241:ARG:HD2	2.20	0.41
3:A:502:ATP:O1A	3:A:502:ATP:O3B	2.38	0.41
1:B:176:THR:O	1:B:176:THR:HG22	2.19	0.41
1:A:40:ARG:NH2	1:A:407:ASP:OD1	2.54	0.41
1:B:38:VAL:CG1	1:B:148:ASP:HB2	2.44	0.41
1:B:70:ARG:C	1:B:72:ASN:H	2.24	0.41
1:B:201:LEU:HD23	1:B:206:ILE:CG1	2.50	0.41
1:A:19:GLY:HA3	3:A:502:ATP:O2B	2.21	0.41
1:A:329:PRO:O	1:A:331:PRO:CD	2.68	0.41
1:B:295:VAL:HG22	1:B:373:ILE:HD11	2.02	0.41
1:B:45:ARG:C	1:B:47:ASN:N	2.74	0.41
1:A:195:MET:HE2	1:A:195:MET:HB3	1.32	0.41
1:A:263:GLU:OE1	1:A:263:GLU:HA	2.21	0.41
1:A:414:LYS:HA	1:A:414:LYS:HD2	1.83	0.41
1:B:355:LYS:O	1:B:359:GLU:HG3	2.21	0.41
1:A:16:ARG:O	1:A:16:ARG:HD3	2.21	0.41
1:A:182:LYS:HZ2	1:B:132:ASN:HB2	1.85	0.41
1:A:280:ASP:OD1	1:A:280:ASP:N	2.54	0.41
1:B:15:TYR:HA	1:B:25:LEU:HD22	2.03	0.41
1:A:5:LEU:H	1:A:5:LEU:CD1	2.32	0.41
1:A:15:TYR:CE2	1:A:126:ARG:HG2	2.56	0.41
1:A:122:VAL:HG23	1:A:126:ARG:HD2	2.03	0.40
1:A:389:TYR:C	1:A:389:TYR:CD1	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:HD3	1:B:252:GLY:O	2.21	0.40
1:A:5:LEU:CD1	1:A:108:VAL:CG2	3.00	0.40
1:A:218:PHE:CZ	1:A:301:LEU:HD22	2.56	0.40
1:B:169:PRO:HB2	1:B:218:PHE:CE2	2.57	0.40
1:A:97:LEU:CD1	1:A:307:ILE:HD13	2.50	0.40
1:B:-2:GLN:NE2	1:B:-1:GLY:N	2.68	0.40
1:A:321:CYS:O	1:A:325:ILE:HG12	2.22	0.40
1:A:408:LEU:HD23	1:A:408:LEU:HA	1.68	0.40
1:B:179:PHE:CE1	1:B:345:LEU:HD22	2.57	0.40
1:B:226:LEU:CD1	1:B:292:SER:CB	2.99	0.40
1:B:269:GLU:HG3	1:B:283:ARG:HB2	2.03	0.40
1:A:124:LYS:H	1:A:124:LYS:HG3	1.75	0.40
1:A:222:LYS:HB2	1:A:222:LYS:NZ	2.36	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	408/470 (87%)	363 (89%)	35 (9%)	10 (2%)	5 7
1	B	400/470 (85%)	354 (88%)	40 (10%)	6 (2%)	10 15
All	All	808/940 (86%)	717 (89%)	75 (9%)	16 (2%)	7 10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	GLU
1	A	327	ASN
1	A	394	PRO
1	B	343	LEU
1	A	250	LEU

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Mol	Chain	Res	Type
1	A	396	ASN
1	A	71	GLU
1	A	72	ASN
1	B	139	SER
1	B	298	SER
1	B	392	LEU
1	A	123	THR
1	A	311	ASP
1	B	46	ARG
1	A	332	ILE
1	B	249	ILE

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	375/415 (90%)	342 (91%)	33 (9%)	10 14
1	B	368/415 (89%)	329 (89%)	39 (11%)	6 10
All	All	743/830 (90%)	671 (90%)	72 (10%)	8 11

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	LYS
1	A	14	ILE
1	A	47	ASN
1	A	60	VAL
1	A	68	LEU
1	A	70	ARG
1	A	71	GLU
1	A	109	SER
1	A	125	GLN
1	A	150	SER
1	A	161	ASP

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Mol	Chain	Res	Type
1	A	165	VAL
1	A	182	LYS
1	A	183	GLU
1	A	185	MET
1	A	208	GLU
1	A	222	LYS
1	A	244	LEU
1	A	263	GLU
1	A	264	ILE
1	A	285	GLU
1	A	319	ILE
1	A	328	GLN
1	A	342	GLU
1	A	352	GLU
1	A	368	ASP
1	A	388	ASP
1	A	389	TYR
1	A	391	SER
1	A	400	ASP
1	A	434	GLN
1	A	435	LYS
1	B	-5	VAL
1	B	-2	GLN
1	B	16	ARG
1	B	45	ARG
1	B	47	ASN
1	B	76	ILE
1	B	85	GLU
1	B	93	ILE
1	B	100	LYS
1	B	103	ASP
1	B	107	ARG
1	B	123	THR
1	B	128	LEU
1	B	146	LEU
1	B	162	CYS
1	B	165	VAL
1	B	194	LYS
1	B	196	HIS
1	B	208	GLU
1	B	215	LEU
1	B	244	LEU

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Mol	Chain	Res	Type
1	B	264	ILE
1	B	277	GLN
1	B	284	THR
1	B	301	LEU
1	B	325	ILE
1	B	343	LEU
1	B	345	LEU
1	B	352	GLU
1	B	361	LEU
1	B	370	SER
1	B	371	ILE
1	B	393	LYS
1	B	398	THR
1	B	400	ASP
1	B	414	LYS
1	B	416	MET
1	B	434	GLN
1	B	437	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	91	ASN
1	A	149	HIS
1	A	196	HIS
1	A	404	HIS
1	A	434	GLN
1	B	91	ASN
1	B	132	ASN
1	B	135	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
7	B3P	B	506	-	18,18,18	0.59	0	21,23,23	1.08	1 (4%)
6	EDO	A	505	-	3,3,3	0.60	0	2,2,2	0.22	0
6	EDO	A	506	-	3,3,3	0.57	0	2,2,2	0.07	0
3	ATP	B	502	4	26,33,33	1.05	2 (7%)	31,52,52	1.36	3 (9%)
3	ATP	A	502	4	26,33,33	1.06	2 (7%)	31,52,52	1.40	4 (12%)
2	K7V	B	501	-	32,32,32	0.80	1 (3%)	48,53,53	1.17	4 (8%)
2	K7V	A	501	-	32,32,32	1.02	3 (9%)	48,53,53	1.08	1 (2%)
6	EDO	B	507	-	3,3,3	0.48	0	2,2,2	0.28	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
7	B3P	B	506	-	-	17/28/28/28	-
6	EDO	A	505	-	-	0/1/1/1	-
6	EDO	A	506	-	-	0/1/1/1	-
3	ATP	B	502	4	-	4/18/38/38	0/3/3/3
3	ATP	A	502	4	-	0/18/38/38	0/3/3/3
2	K7V	B	501	-	-	9/25/49/49	0/1/1/1
2	K7V	A	501	-	-	6/25/49/49	0/1/1/1
6	EDO	B	507	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ATP	O4'-C1'	2.71	1.44	1.41
2	A	501	K7V	P5-O15	2.67	1.64	1.59
3	B	502	ATP	C5-C4	2.60	1.47	1.40
3	A	502	ATP	C5-C4	2.38	1.47	1.40
2	A	501	K7V	P3-O13	2.31	1.63	1.59
3	B	502	ATP	C2-N3	2.19	1.35	1.32
2	A	501	K7V	P6-O16	2.10	1.63	1.59
2	B	501	K7V	P5-O15	2.09	1.63	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	ATP	N3-C2-N1	-4.19	122.12	128.68
3	B	502	ATP	PA-O3A-PB	-3.85	119.60	132.83
2	B	501	K7V	O11-P1-O21	-2.80	98.58	109.39
7	B	506	B3P	C2-N2-C8	-2.70	112.24	116.08
3	A	502	ATP	PA-O3A-PB	-2.66	123.68	132.83
3	B	502	ATP	N3-C2-N1	-2.58	124.65	128.68
2	B	501	K7V	O14-C4-C3	-2.35	103.14	108.69
3	B	502	ATP	C4-C5-N7	-2.34	106.96	109.40
3	A	502	ATP	C3'-C2'-C1'	2.12	104.18	100.98
2	B	501	K7V	O13-P3-O43	-2.11	101.27	109.39
3	A	502	ATP	C2-N1-C6	2.07	122.30	118.75
2	B	501	K7V	O34-P4-O24	2.03	115.41	107.64
2	A	501	K7V	C2-C3-C4	-2.02	107.04	111.66

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	K7V	C4-O14-P4-O44
2	B	501	K7V	C1-O11-P1-O21
2	B	501	K7V	C1-O11-P1-O41
3	B	502	ATP	O4'-C4'-C5'-O5'
7	B	506	B3P	C5-C4-N1-C3
7	B	506	B3P	C6-C4-N1-C3
7	B	506	B3P	N1-C4-C5-O4
7	B	506	B3P	C6-C4-C5-O4
7	B	506	B3P	C7-C4-C5-O4
7	B	506	B3P	N1-C4-C7-O6
7	B	506	B3P	C5-C4-C7-O6
7	B	506	B3P	C6-C4-C7-O6

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Mol	Chain	Res	Type	Atoms
7	B	506	B3P	N2-C8-C9-O1
7	B	506	B3P	C11-C8-C9-O1
6	B	507	EDO	O1-C1-C2-O2
7	B	506	B3P	C3-C1-C2-N2
7	B	506	B3P	C9-C8-N2-C2
7	B	506	B3P	C10-C8-N2-C2
7	B	506	B3P	C10-C8-C9-O1
2	B	501	K7V	C3-O13-P3-O23
7	B	506	B3P	C7-C4-N1-C3
7	B	506	B3P	C2-C1-C3-N1
2	A	501	K7V	C2-C3-O13-P3
3	B	502	ATP	PG-O3B-PB-O2B
3	B	502	ATP	PA-O3A-PB-O1B
2	A	501	K7V	C6-O16-P6-O46
2	B	501	K7V	C3-O13-P3-O43
2	B	501	K7V	C5-O15-P5-O25
3	B	502	ATP	C3'-C4'-C5'-O5'
2	A	501	K7V	C5-O15-P5-O35
2	A	501	K7V	C6-O16-P6-O36
2	A	501	K7V	C4-C3-O13-P3
2	B	501	K7V	C3-O13-P3-O33
2	B	501	K7V	C5-O15-P5-O35
2	B	501	K7V	C5-O15-P5-O45
2	B	501	K7V	C6-O16-P6-O26
7	B	506	B3P	C11-C8-N2-C2

There are no ring outliers.

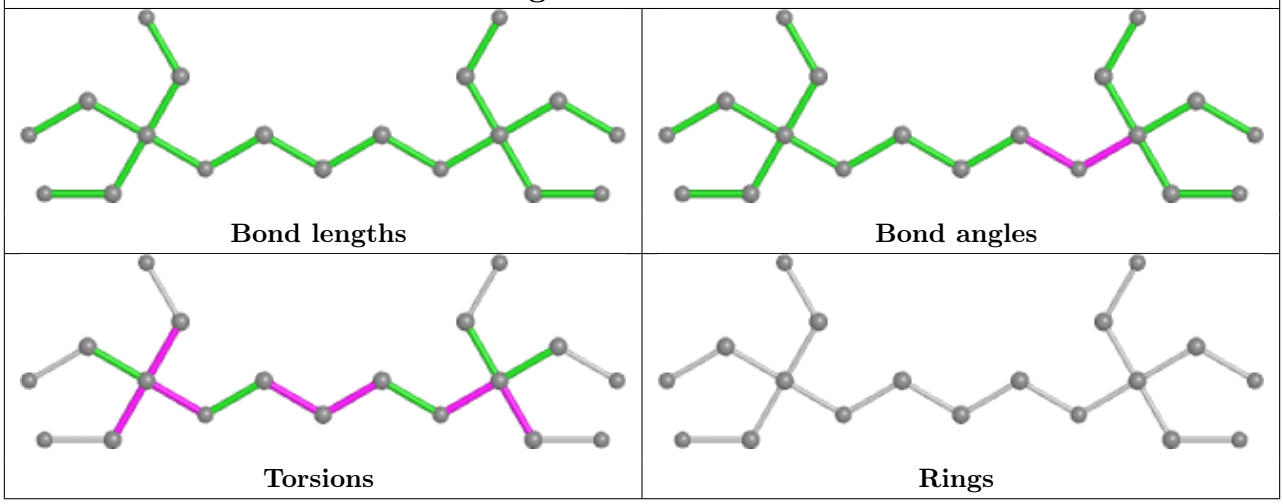
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	506	B3P	2	0
3	B	502	ATP	6	0
3	A	502	ATP	2	0

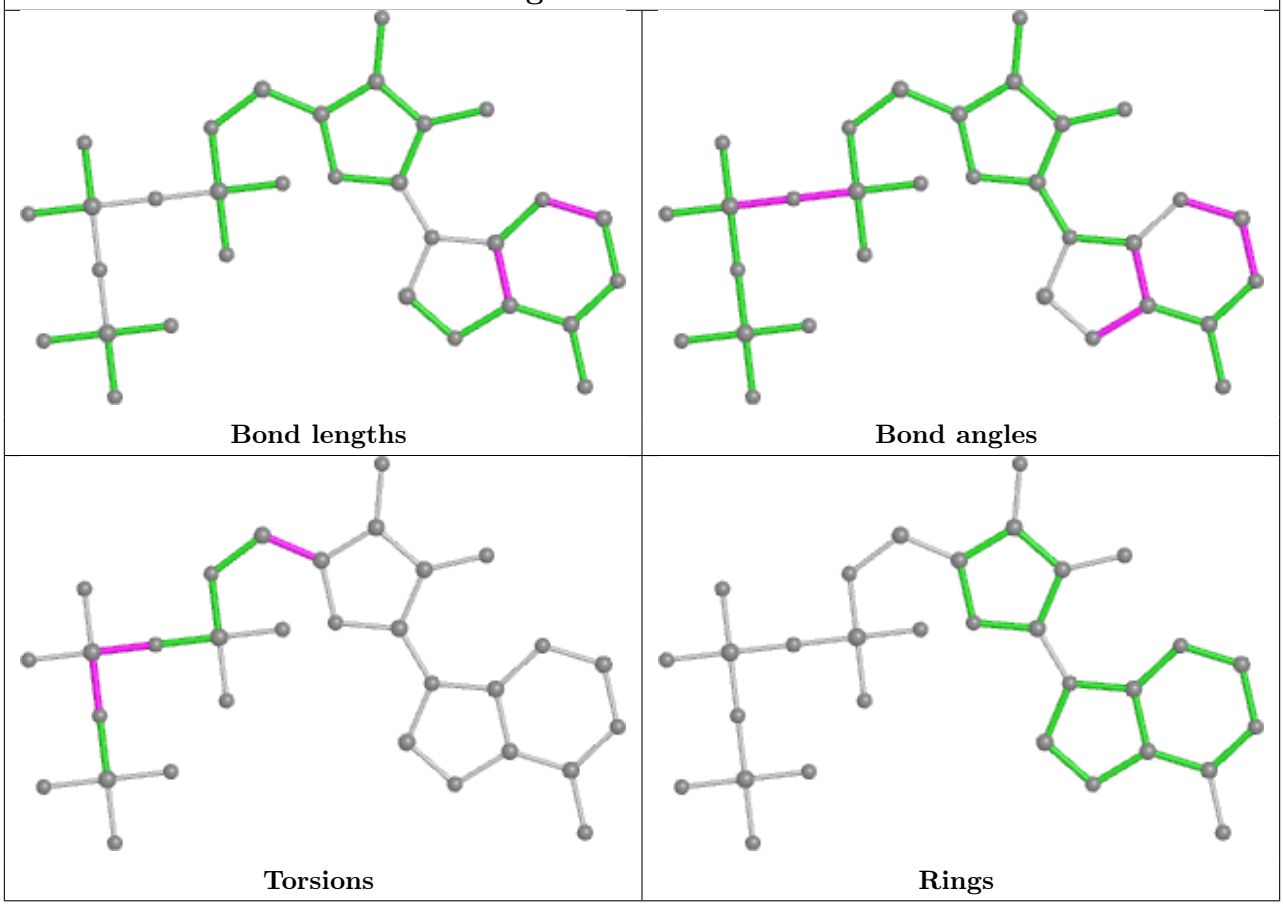
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

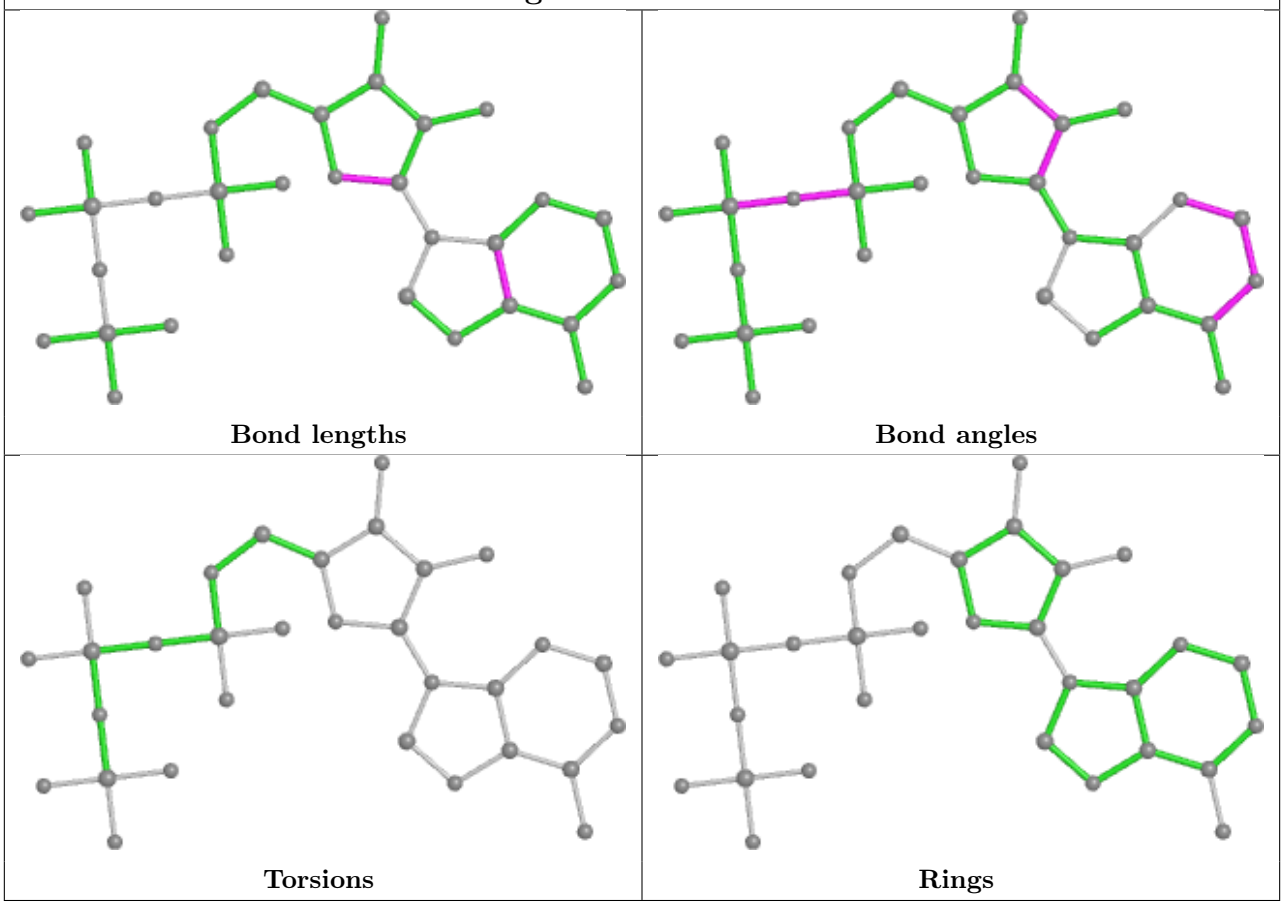
Ligand B3P B 506



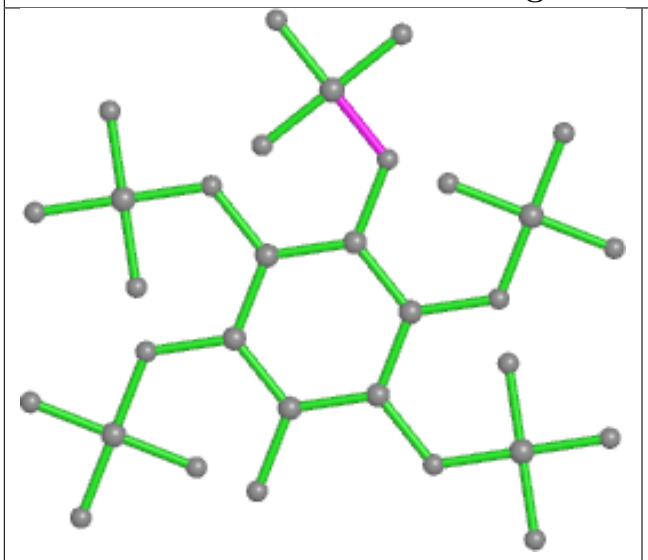
Ligand ATP B 502



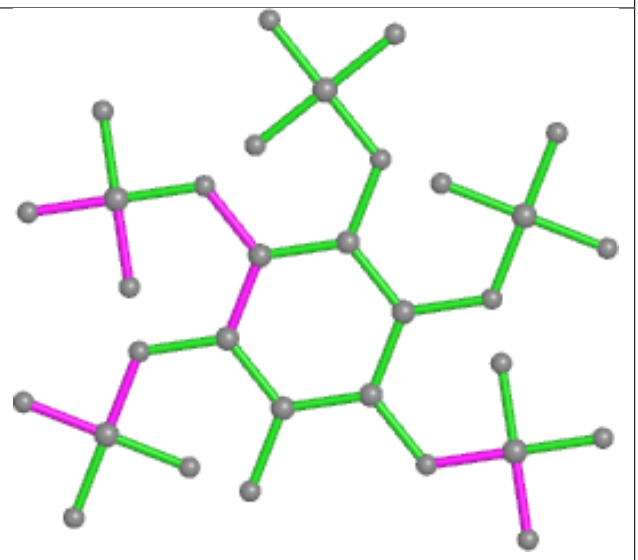
Ligand ATP A 502



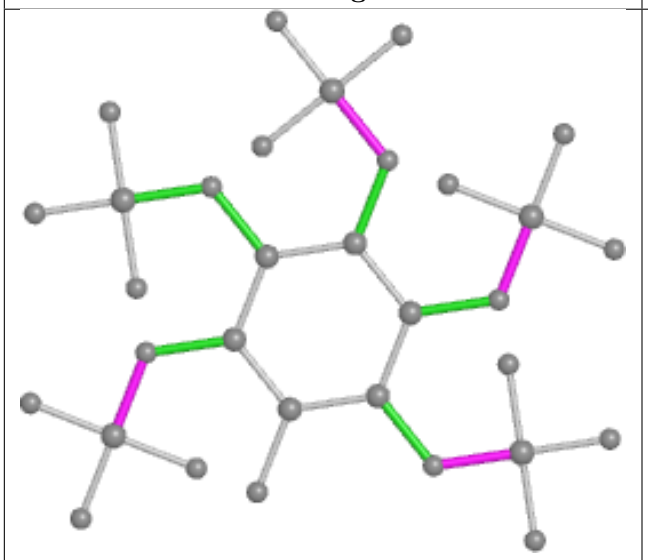
Ligand K7V B 501



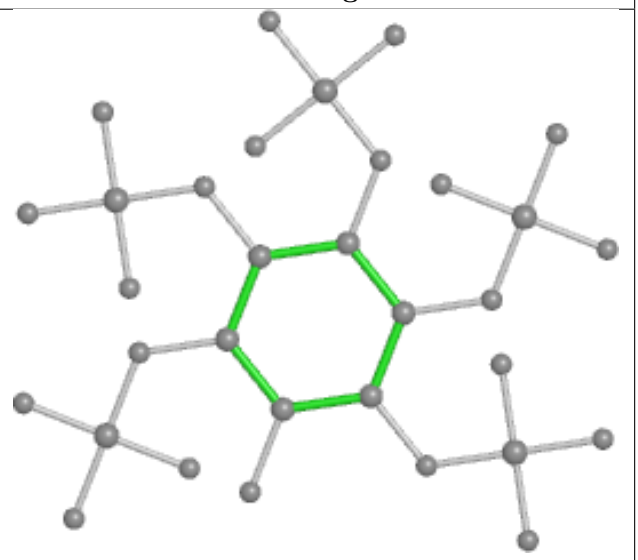
Bond lengths



Bond angles

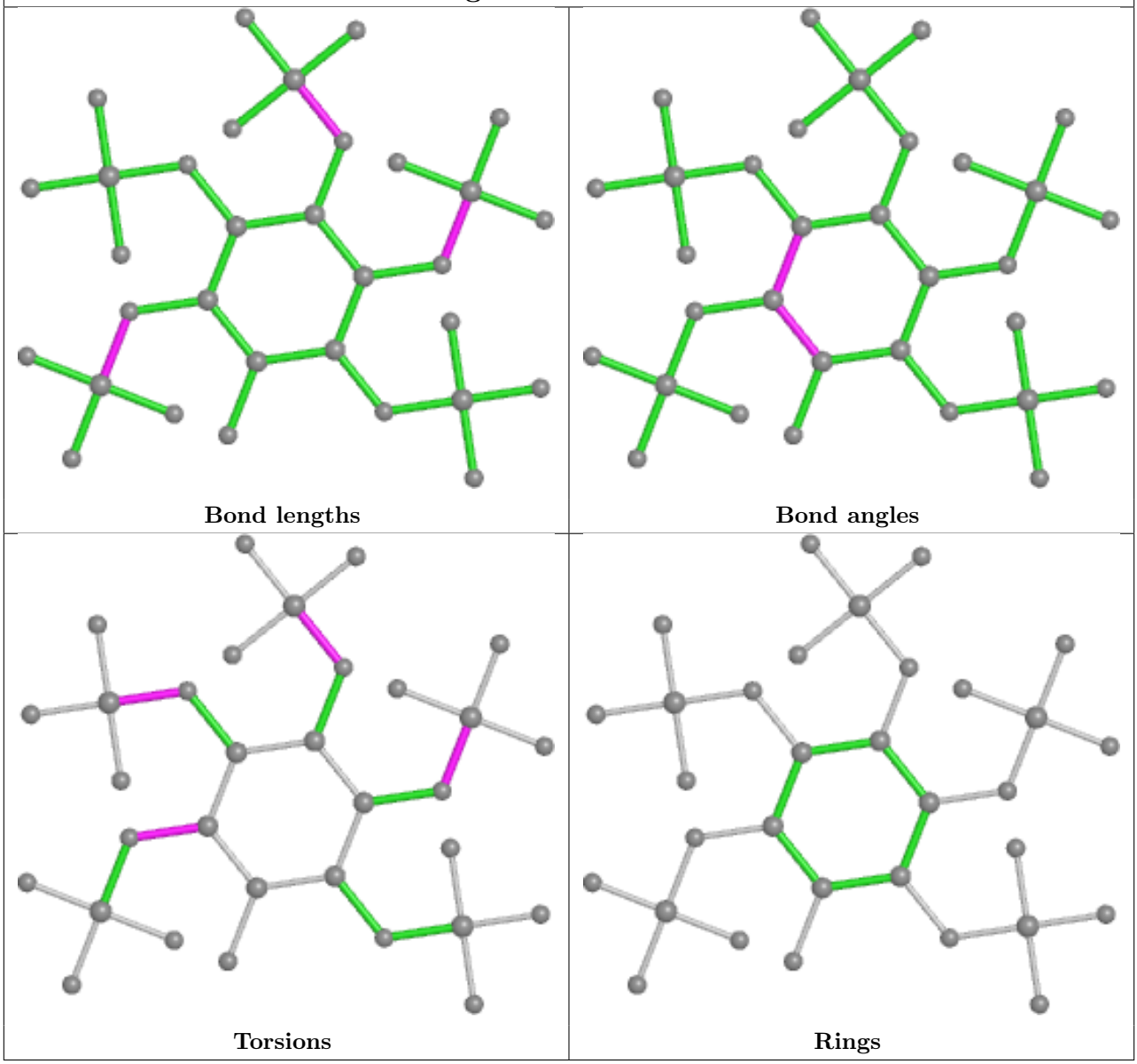


Torsions



Rings

Ligand K7V A 501



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	420/470 (89%)	0.06	14 (3%)	46	43	25, 51, 83, 102	0
1	B	410/470 (87%)	-0.01	14 (3%)	45	41	26, 51, 83, 95	0
All	All	830/940 (88%)	0.03	28 (3%)	45	41	25, 51, 83, 102	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	LEU	3.6
1	A	343	LEU	3.5
1	A	387	GLY	3.5
1	B	30	SER	3.4
1	B	124	LYS	3.4
1	B	167	ILE	3.2
1	B	47	ASN	3.2
1	A	58	VAL	3.2
1	B	391	SER	3.1
1	A	57	VAL	2.9
1	A	48	ASP	2.8
1	B	9	ASP	2.8
1	A	274	GLY	2.7
1	A	56	GLY	2.7
1	B	389	TYR	2.7
1	A	335	GLU	2.5
1	A	342	GLU	2.4
1	B	27	TYR	2.4
1	B	10	ALA	2.4
1	B	48	ASP	2.4
1	B	223	GLU	2.3
1	B	436	ALA	2.3
1	A	379	ASN	2.3
1	A	277	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	55	ASN	2.2
1	A	399	PHE	2.1
1	A	329	PRO	2.1
1	B	32	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

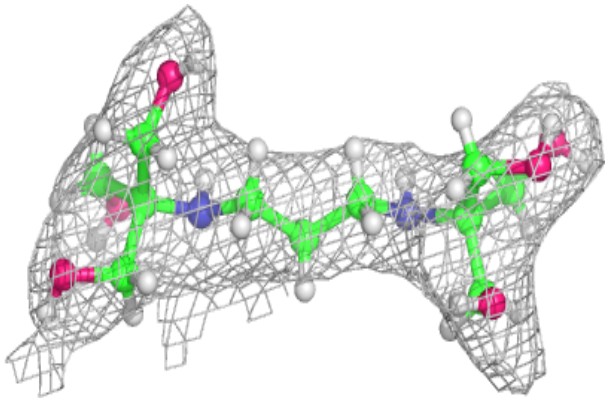
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

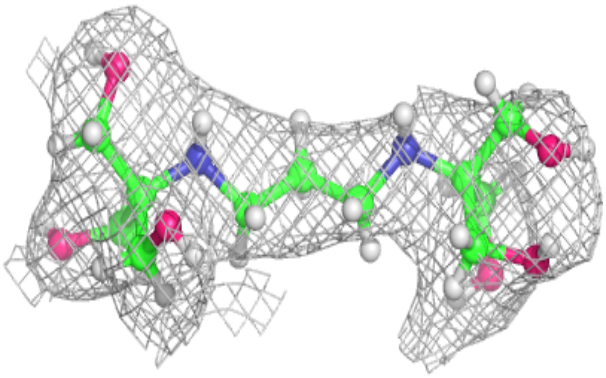
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	506	4/4	0.78	0.22	59,71,80,80	0
6	EDO	A	505	4/4	0.83	0.17	51,61,69,69	0
7	B3P	B	506	19/19	0.90	0.18	39,54,77,82	0
6	EDO	B	507	4/4	0.93	0.19	53,64,66,67	0
2	K7V	A	501	32/32	0.95	0.14	38,55,69,77	0
3	ATP	A	502	31/31	0.96	0.22	37,49,59,72	0
3	ATP	B	502	31/31	0.96	0.20	43,57,68,75	0
4	MG	B	503	1/1	0.97	0.35	44,44,44,44	0
4	MG	B	504	1/1	0.97	0.26	45,45,45,45	0
2	K7V	B	501	32/32	0.97	0.12	37,48,58,61	0
5	ZN	A	504	1/1	0.99	0.08	48,48,48,48	0
5	ZN	B	505	1/1	0.99	0.07	44,44,44,44	0
4	MG	A	503	1/1	0.99	0.35	44,44,44,44	0

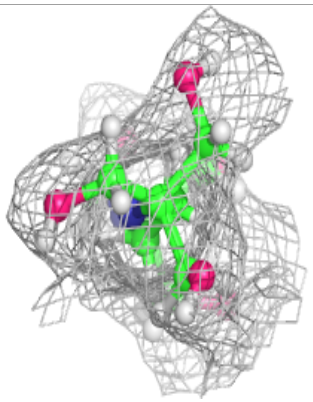
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P B 506:

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

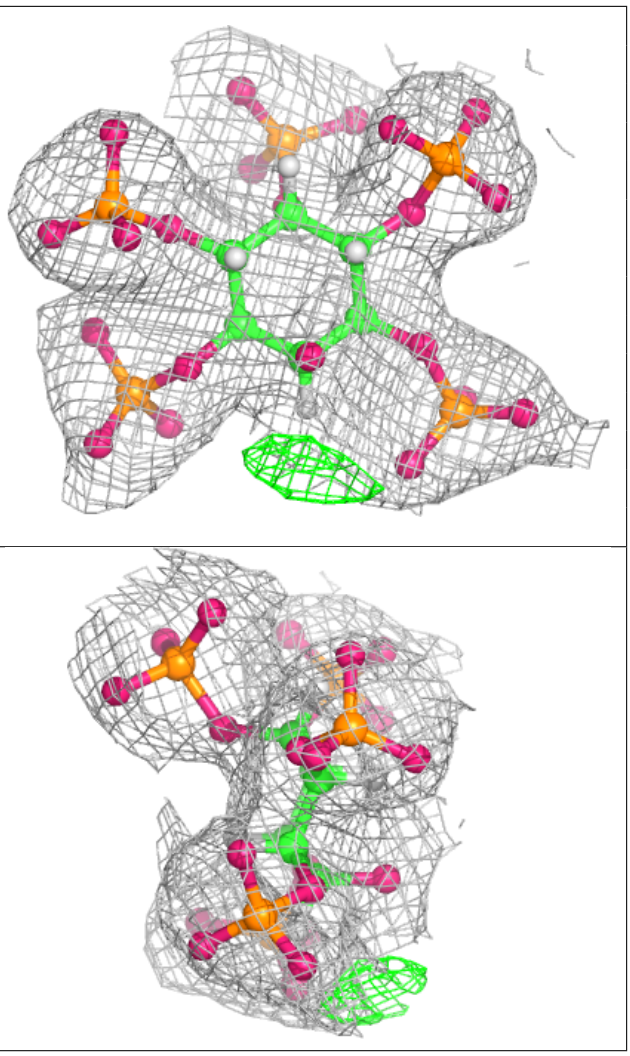






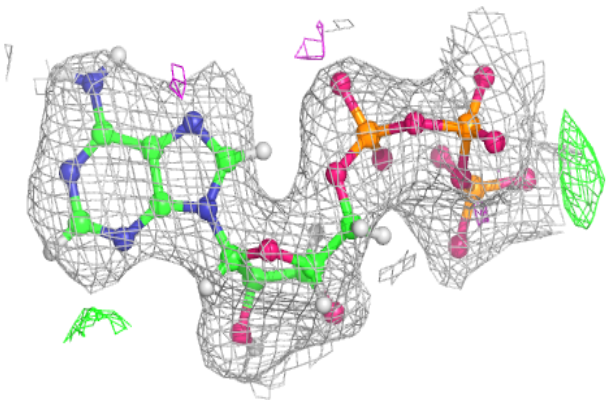
Electron density around K7V A 501:

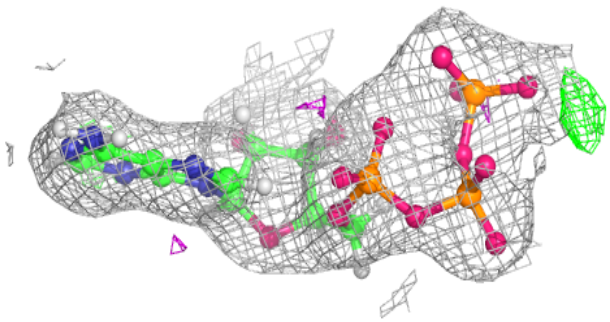
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

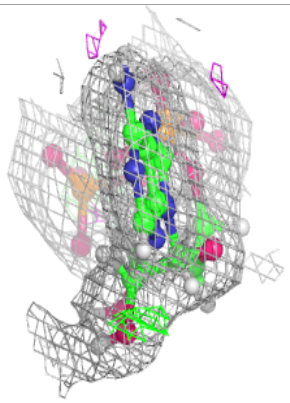


Electron density around ATP A 502:

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

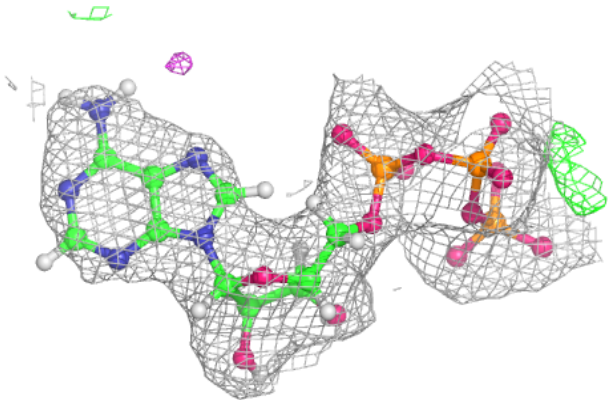


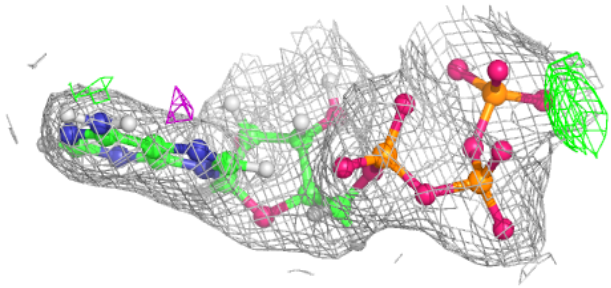


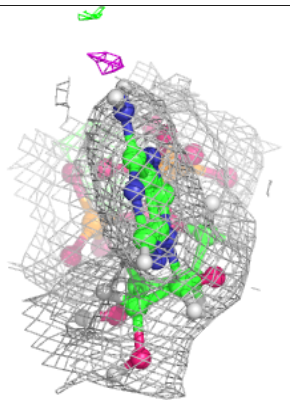


Electron density around ATP B 502:

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

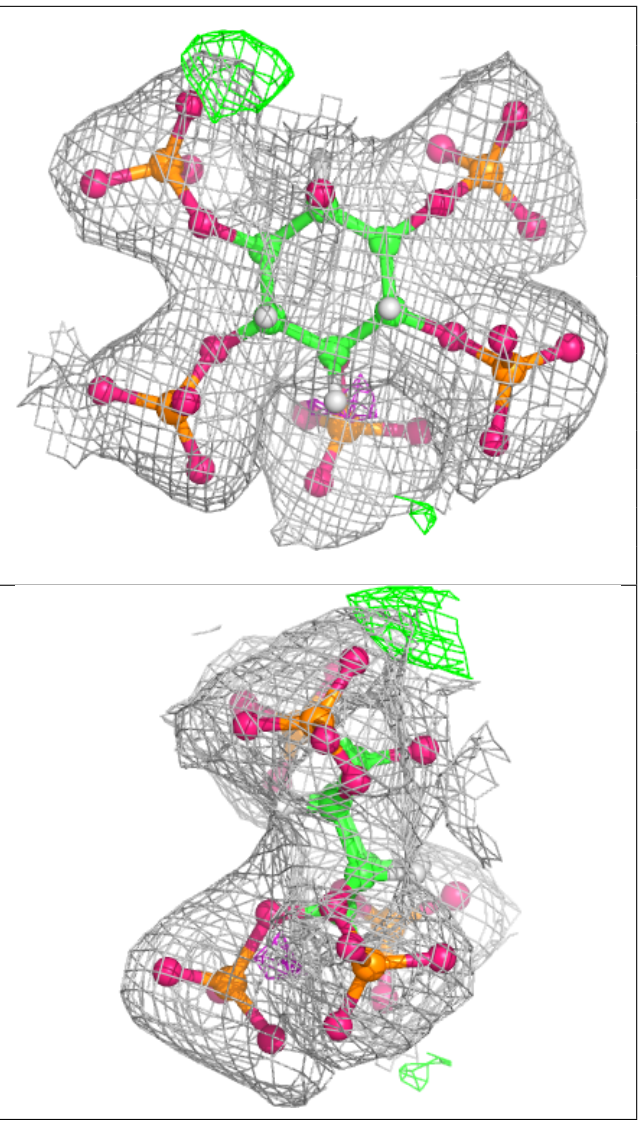






Electron density around K7V B 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.