Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 02:07 PM EDT

PDB ID	:	8DB3
Title	:	Crystal structure of KaiC with truncated C-terminal coiled-coil domain
Authors	:	Padua, R.A.P.; Grant, T.; Pitsawong, W.; Hoemberger, M.S.; Otten, R.; Bradshaw, N.; Grigorieff, N.; Kern, D.
Deposited on	:	2022-06-14
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

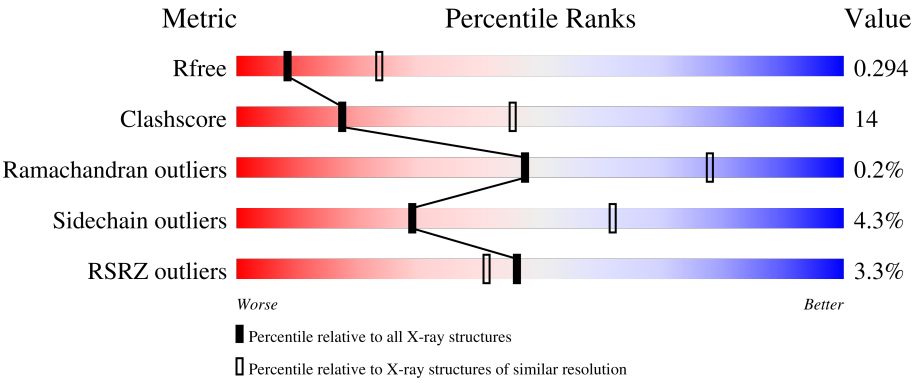
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	490	5% 63% 24% • 11%
1	C	490	2% 63% 27% • 9%
2	B	490	2% 69% 19% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20488 atoms, of which 10195 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.

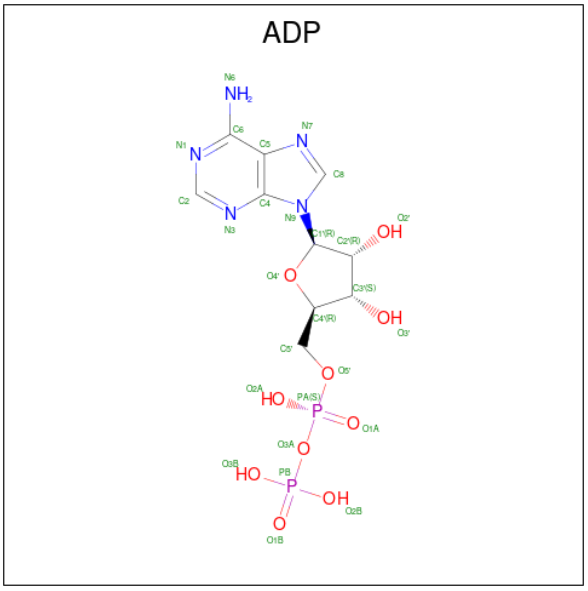
- Molecule 1 is a protein called Circadian clock protein KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	H	N	O	S	0	0	0
			6671	2114	3335	590	616	16			
1	C	446	Total	C	H	N	O	S	0	0	0
			6848	2168	3423	603	638	16			

- Molecule 2 is a protein called Circadian clock protein KaiC.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	439	Total	C	H	N	O	P	S	0	0	0
			6738	2134	3368	590	628	1	17			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		

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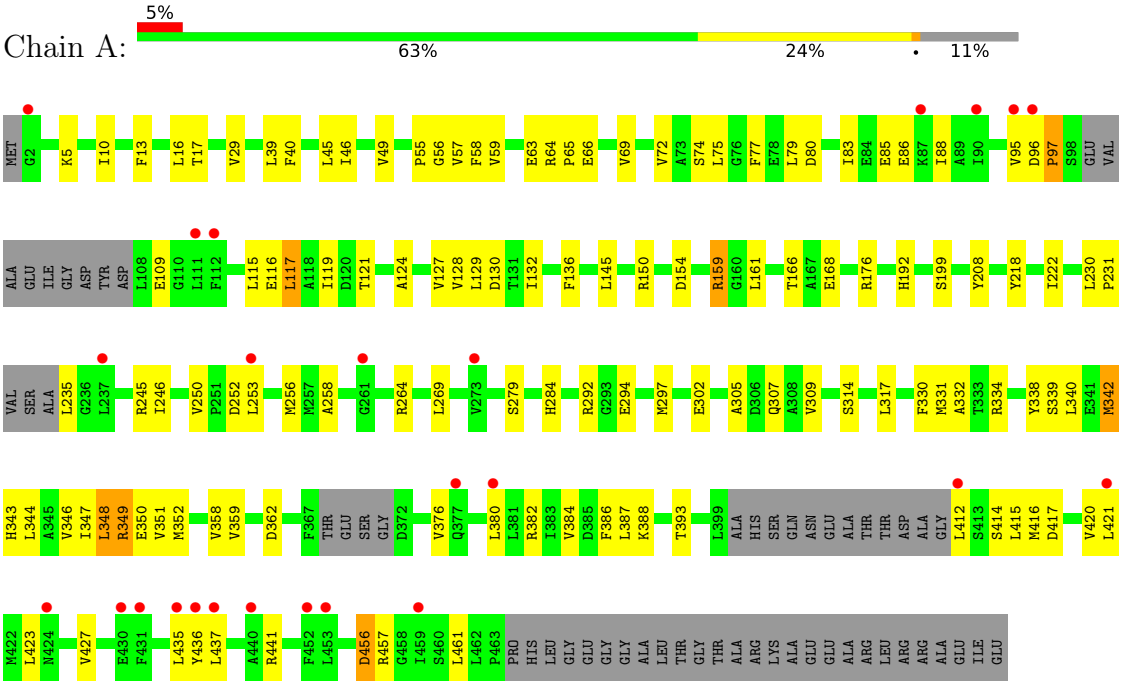
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
3	B	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
3	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
3	C	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
3	C	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

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.

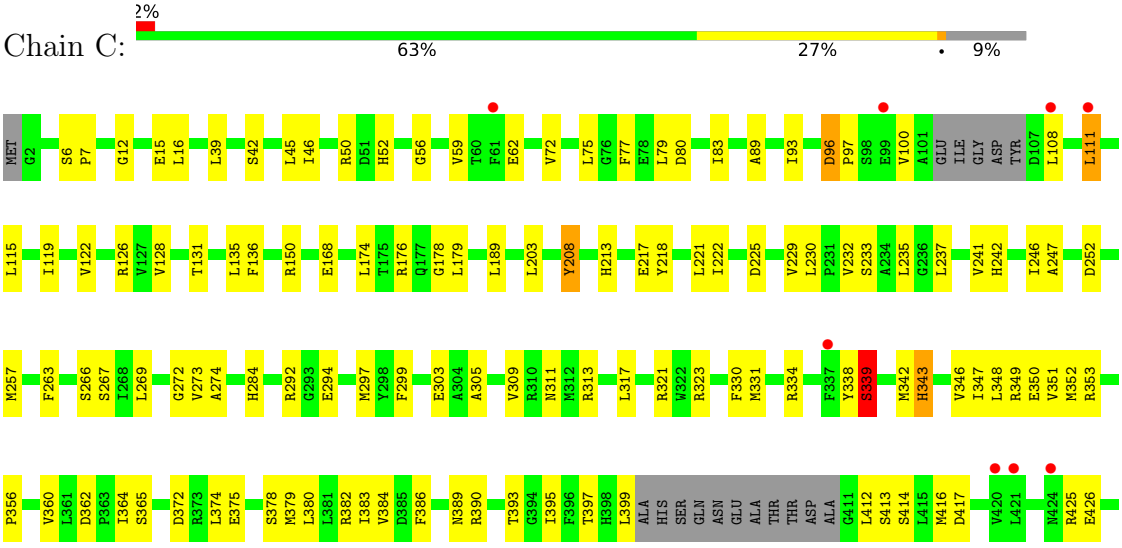
• Molecule 1: Circadian clock protein KaiC

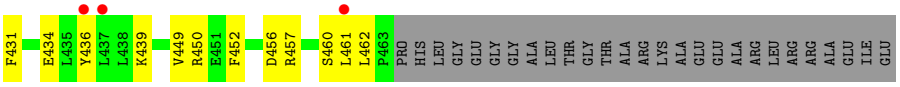
Chain A:



• Molecule 1: Circadian clock protein KaiC

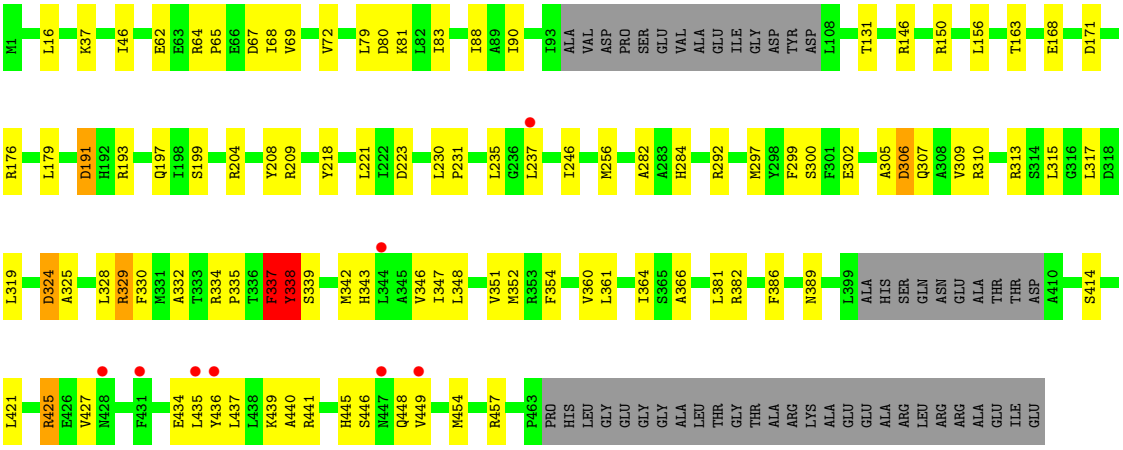
Chain C:





• Molecule 2: Circadian clock protein KaiC

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	94.06Å 197.28Å 150.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.75 – 2.90 59.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.75-2.90) 90.4 (59.75-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.236 , 0.295 0.236 , 0.294	Depositor DCC
R_{free} test set	1999 reflections (6.37%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 31.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	20488	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	1/3391 (0.0%)	0.55	0/4573
1	C	0.29	0/3483	0.56	0/4702
2	B	0.35	2/3416 (0.1%)	0.63	5/4609 (0.1%)
All	All	0.32	3/10290 (0.0%)	0.58	5/13884 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLU	CG-CD	-6.16	1.42	1.51
2	B	337	PHE	CD1-CE1	-5.24	1.28	1.39
2	B	337	PHE	CG-CD1	-5.13	1.31	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	337	PHE	CB-CG-CD1	-12.46	112.08	120.80
2	B	337	PHE	CB-CG-CD2	10.03	127.82	120.80
2	B	338	TYR	CG-CD1-CE1	8.09	127.77	121.30
2	B	338	TYR	CD1-CE1-CZ	-5.74	114.63	119.80
2	B	338	TYR	CZ-CE2-CD2	5.68	124.91	119.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3336	3335	3334	100	0
1	C	3425	3423	3423	101	0
2	B	3370	3368	3368	97	0
3	A	54	23	24	1	0
3	B	54	23	24	0	0
3	C	54	23	24	1	0
All	All	10293	10195	10197	282	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 14.

All (282) 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)
2:B:446:SER:OG	2:B:448:GLN:OE1	1.65	1.12
1:C:292:ARG:NH1	1:C:294:GLU:OE2	1.87	1.08
2:B:338:TYR:CD1	2:B:342:MET:HE3	1.90	1.06
2:B:337:PHE:HE1	2:B:338:TYR:CE1	1.84	0.95
1:C:15:GLU:OE1	1:C:233:SER:OG	1.86	0.93
1:C:42:SER:O	1:C:46:ILE:HD13	1.70	0.91
2:B:337:PHE:HE1	2:B:338:TYR:CD1	1.94	0.84
2:B:338:TYR:CD1	2:B:342:MET:CE	2.61	0.81
2:B:230:LEU:HD12	2:B:231:PRO:HD2	1.66	0.78
1:A:421:LEU:HD23	1:A:436:TYR:HD2	1.50	0.77
1:C:450:ARG:NH1	1:C:462:LEU:O	2.17	0.76
2:B:80:ASP:HA	2:B:83:ILE:HD12	1.67	0.76
2:B:221:LEU:HD21	2:B:342:MET:SD	2.27	0.74
1:A:344:LEU:O	1:A:348:LEU:HD23	1.86	0.74
1:A:302:GLU:OE2	2:B:441:ARG:NH2	2.22	0.73
1:A:45:LEU:HD13	1:A:128:VAL:HG23	1.71	0.73
2:B:337:PHE:CE1	2:B:338:TYR:CZ	2.78	0.72
1:C:168:GLU:OE1	1:C:176:ARG:NH2	2.21	0.72
2:B:337:PHE:CE1	2:B:338:TYR:CE1	2.75	0.72
1:A:168:GLU:OE1	1:A:176:ARG:NH2	2.22	0.72
1:A:332:ALA:HB1	2:B:237:LEU:HD12	1.72	0.72
1:A:109:GLU:N	1:A:109:GLU:OE1	2.24	0.70
2:B:319:LEU:HD12	2:B:328:LEU:HD21	1.74	0.70
1:A:284:HIS:ND1	1:A:317:LEU:HD11	2.06	0.69
2:B:337:PHE:HE1	2:B:338:TYR:CZ	2.09	0.69
1:A:46:ILE:HD11	1:A:79:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ALA:HB2	1:C:122:VAL:HG21	1.75	0.69
2:B:307:GLN:NE2	1:C:417:ASP:OD1	2.26	0.69
1:A:421:LEU:HD23	1:A:436:TYR:CD2	2.28	0.69
2:B:337:PHE:CE1	2:B:338:TYR:CD1	2.79	0.68
1:A:246:ILE:CG2	1:A:264:ARG:HD3	2.24	0.68
1:C:232:VAL:HG22	1:C:235:LEU:HD13	1.77	0.67
1:C:42:SER:O	1:C:46:ILE:CD1	2.43	0.67
1:C:450:ARG:HB3	1:C:461:LEU:HD23	1.77	0.67
1:C:378:SER:OG	1:C:382:ARG:NH2	2.28	0.66
1:C:59:VAL:HG21	1:C:115:LEU:CD2	2.25	0.66
1:A:116:GLU:HA	1:A:119:ILE:HD12	1.76	0.66
1:C:436:TYR:CE1	1:C:449:VAL:HG22	2.30	0.66
2:B:168:GLU:OE1	2:B:176:ARG:NH2	2.29	0.65
1:A:344:LEU:HD21	1:A:382:ARG:HD2	1.78	0.65
1:C:348:LEU:O	1:C:352:MET:HG3	1.97	0.65
2:B:332:ALA:HB1	1:C:237:LEU:HD12	1.80	0.64
1:A:117:LEU:O	1:A:121:THR:HG23	1.98	0.64
1:C:364:ILE:HD11	1:C:380:LEU:HD11	1.80	0.63
1:C:330:PHE:O	1:C:331:MET:HE2	1.99	0.63
2:B:348:LEU:HD22	2:B:386:PHE:CG	2.33	0.63
1:C:272:GLY:O	1:C:399:LEU:HD12	1.98	0.62
1:C:235:LEU:O	1:C:389:ASN:ND2	2.32	0.62
1:A:253:LEU:HD12	1:A:256:MET:HE2	1.81	0.62
2:B:282:ALA:HB1	2:B:360:VAL:HG11	1.82	0.62
2:B:315:LEU:HD11	2:B:454:MET:HE3	1.83	0.61
2:B:305:ALA:O	2:B:309:VAL:HG23	2.01	0.61
2:B:282:ALA:HB1	2:B:360:VAL:CG1	2.31	0.61
2:B:324:ASP:OD1	2:B:325:ALA:N	2.34	0.60
1:C:174:LEU:HD23	1:C:189:LEU:HD13	1.83	0.60
1:A:65:PRO:O	1:A:69:VAL:HG23	2.02	0.60
1:A:253:LEU:HD12	1:A:256:MET:CE	2.32	0.59
2:B:315:LEU:HD11	2:B:454:MET:CE	2.31	0.59
1:C:232:VAL:CG2	1:C:235:LEU:HD13	2.32	0.59
1:C:59:VAL:HG21	1:C:115:LEU:HD21	1.82	0.59
1:C:339:SER:O	1:C:343:HIS:N	2.33	0.59
1:A:115:LEU:O	1:A:119:ILE:HD12	2.02	0.59
1:C:413:SER:O	1:C:439:LYS:NZ	2.33	0.59
1:A:334:ARG:HD2	2:B:381:LEU:HD13	1.83	0.58
2:B:80:ASP:CA	2:B:83:ILE:HD12	2.34	0.58
1:C:450:ARG:CB	1:C:461:LEU:HD23	2.33	0.58
2:B:338:TYR:CE1	2:B:342:MET:HE3	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:LEU:O	2:B:83:ILE:HD12	2.03	0.58
1:C:342:MET:O	1:C:346:VAL:HG13	2.01	0.58
1:C:269:LEU:HB2	1:C:416:MET:HG3	1.86	0.57
1:C:297:MET:HE1	1:C:351:VAL:HA	1.85	0.57
1:A:342:MET:O	1:A:346:VAL:HG23	2.05	0.57
1:A:338:TYR:O	1:A:339:SER:HB3	2.04	0.57
1:A:314:SER:OG	3:A:601:ADP:N7	2.32	0.56
1:C:96:ASP:HB3	1:C:97:PRO:CD	2.36	0.56
1:C:348:LEU:HD22	1:C:386:PHE:CG	2.40	0.56
2:B:335:PRO:HG2	2:B:366:ALA:HB1	1.88	0.56
1:A:343:HIS:O	1:A:347:ILE:HD12	2.06	0.55
2:B:338:TYR:CE1	2:B:342:MET:CE	2.90	0.55
2:B:80:ASP:HA	2:B:83:ILE:CD1	2.37	0.55
1:C:59:VAL:HG13	1:C:93:ILE:HD12	1.87	0.55
1:C:89:ALA:HB2	1:C:122:VAL:CG2	2.37	0.55
2:B:337:PHE:HD1	2:B:338:TYR:CD2	2.24	0.54
1:A:192:HIS:CD2	1:A:199:SER:HB3	2.42	0.54
1:A:359:VAL:HB	1:A:387:LEU:HD21	1.89	0.54
2:B:338:TYR:HD1	2:B:342:MET:CE	2.21	0.54
1:A:380:LEU:O	1:A:384:VAL:HG23	2.08	0.53
2:B:171:ASP:OD1	2:B:171:ASP:N	2.40	0.53
1:A:331:MET:SD	1:A:350:GLU:HG2	2.49	0.53
1:A:168:GLU:OE1	2:B:146:ARG:NH2	2.42	0.53
1:A:16:LEU:HD13	1:A:218:TYR:CD2	2.44	0.53
2:B:425:ARG:NH1	2:B:434:GLU:OE2	2.42	0.53
1:C:42:SER:C	1:C:46:ILE:HD13	2.29	0.53
1:C:96:ASP:HB3	1:C:97:PRO:HD3	1.89	0.53
1:C:115:LEU:O	1:C:119:ILE:HD13	2.09	0.53
1:C:267:SER:HB3	1:C:416:MET:SD	2.49	0.52
2:B:302:GLU:OE1	1:C:414:SER:OG	2.27	0.52
1:C:221:LEU:HD21	1:C:342:MET:SD	2.49	0.52
1:A:79:LEU:HG	1:A:83:ILE:HD11	1.91	0.52
2:B:313:ARG:NH1	2:B:313:ARG:HB3	2.24	0.52
2:B:62:GLU:HB2	2:B:131:THR:HG21	1.90	0.52
2:B:337:PHE:CD1	2:B:338:TYR:CE2	2.98	0.52
2:B:337:PHE:CD1	2:B:338:TYR:CD2	2.98	0.52
1:C:97:PRO:O	1:C:100:VAL:HG22	2.10	0.51
1:A:80:ASP:OD1	1:A:80:ASP:N	2.44	0.51
2:B:319:LEU:HD12	2:B:328:LEU:CD2	2.40	0.51
1:A:116:GLU:CA	1:A:119:ILE:HD12	2.40	0.51
1:A:129:LEU:HB3	1:A:132:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD22	1:A:231:PRO:HD2	1.93	0.51
1:A:130:ASP:OD1	1:A:166:THR:HG21	2.11	0.50
2:B:337:PHE:CE1	2:B:338:TYR:CE2	2.99	0.50
1:C:247:ALA:O	1:C:292:ARG:NH2	2.45	0.50
1:A:297:MET:HE2	1:A:351:VAL:HA	1.94	0.50
1:A:305:ALA:O	1:A:309:VAL:HG13	2.12	0.50
2:B:16:LEU:HD13	2:B:218:TYR:CD2	2.46	0.50
2:B:221:LEU:CD2	2:B:342:MET:SD	2.98	0.50
1:A:59:VAL:HG21	1:A:115:LEU:CD2	2.42	0.50
1:C:379:MET:SD	1:C:383:ILE:HD11	2.52	0.50
1:C:303:GLU:OE2	1:C:311:ASN:ND2	2.45	0.50
1:A:119:ILE:HG23	1:A:124:ALA:HB3	1.93	0.49
1:A:72:VAL:HG23	1:A:75:LEU:HD12	1.93	0.49
1:C:273:VAL:HG12	1:C:274:ALA:N	2.28	0.49
1:A:252:ASP:HB2	1:A:461:LEU:HD13	1.95	0.49
1:A:136:PHE:HB3	1:A:145:LEU:HD11	1.94	0.49
2:B:72:VAL:CG2	2:B:79:LEU:HD12	2.41	0.49
1:A:79:LEU:O	1:A:83:ILE:HD12	2.13	0.49
1:A:380:LEU:HD12	1:A:412:LEU:HD21	1.95	0.49
2:B:334:ARG:HG2	1:C:237:LEU:HD23	1.95	0.49
2:B:324:ASP:OD1	2:B:324:ASP:C	2.51	0.49
1:C:284:HIS:ND1	1:C:317:LEU:HD11	2.28	0.49
1:C:360:VAL:HG22	1:C:395:ILE:HB	1.95	0.49
1:A:349:ARG:NH1	1:A:349:ARG:HG3	2.28	0.49
1:C:59:VAL:HG13	1:C:93:ILE:CD1	2.42	0.48
1:C:456:ASP:OD1	1:C:457:ARG:N	2.45	0.48
1:A:115:LEU:C	1:A:119:ILE:HD12	2.33	0.48
1:A:250:VAL:CG1	1:A:461:LEU:HD11	2.43	0.48
2:B:342:MET:SD	2:B:346:VAL:HG23	2.53	0.48
1:C:46:ILE:HD12	1:C:46:ILE:N	2.29	0.48
1:C:436:TYR:HE1	1:C:449:VAL:HG13	1.77	0.48
1:A:79:LEU:HG	1:A:83:ILE:CD1	2.44	0.48
2:B:440:ALA:HB3	2:B:445:HIS:CD2	2.49	0.48
1:A:256:MET:HE3	1:A:437:LEU:HD12	1.95	0.48
1:A:279:SER:OG	1:A:362:ASP:OD2	2.16	0.48
1:C:349:ARG:O	1:C:353:ARG:HG2	2.14	0.48
1:A:461:LEU:N	1:A:461:LEU:HD12	2.29	0.48
1:A:349:ARG:HG3	1:A:349:ARG:HH11	1.79	0.48
2:B:176:ARG:NH1	1:C:178:GLY:O	2.40	0.48
1:C:299:PHE:CE2	1:C:347:ILE:HD13	2.49	0.48
2:B:46:ILE:HD13	2:B:88:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:ILE:O	2:B:351:VAL:HG23	2.14	0.48
2:B:348:LEU:HD22	2:B:386:PHE:CD2	2.49	0.47
2:B:436:TYR:CE1	2:B:449:VAL:CG1	2.97	0.47
1:A:59:VAL:HB	1:A:129:LEU:HD23	1.96	0.47
1:A:338:TYR:O	1:A:342:MET:SD	2.72	0.47
1:C:222:ILE:HG21	3:C:602:ADP:O4'	2.14	0.47
1:C:305:ALA:O	1:C:309:VAL:HG23	2.13	0.47
1:A:5:LYS:NZ	1:A:17:THR:O	2.45	0.47
2:B:46:ILE:HD13	2:B:88:ILE:CD1	2.44	0.47
1:A:46:ILE:HD12	1:A:77:PHE:HD2	1.78	0.47
1:C:372:ASP:OD1	1:C:372:ASP:C	2.52	0.47
1:A:57:VAL:CG1	1:A:127:VAL:HG22	2.45	0.47
1:A:269:LEU:HB2	1:A:416:MET:HG3	1.96	0.47
1:A:456:ASP:N	1:A:456:ASP:OD1	2.47	0.47
1:C:436:TYR:CE1	1:C:449:VAL:CG2	2.97	0.47
1:A:95:VAL:O	2:B:150:ARG:NH2	2.47	0.47
2:B:197:GLN:HG2	1:C:217:GLU:HB2	1.95	0.47
1:A:388:LYS:NZ	1:A:417:ASP:OD2	2.43	0.47
2:B:79:LEU:HD13	2:B:90:ILE:HD11	1.98	0.47
2:B:246:ILE:HD11	2:B:292:ARG:HH22	1.79	0.47
1:C:50:ARG:NH1	1:C:77:PHE:O	2.48	0.47
2:B:65:PRO:O	2:B:69:VAL:HG23	2.15	0.46
1:C:362:ASP:HA	1:C:397:THR:OG1	2.15	0.46
1:C:380:LEU:O	1:C:384:VAL:HG23	2.15	0.46
1:A:116:GLU:OE1	1:A:159:ARG:NH2	2.47	0.46
1:A:346:VAL:HA	1:A:349:ARG:HG2	1.98	0.46
1:A:96:ASP:O	1:A:97:PRO:C	2.53	0.46
1:C:263:PHE:O	1:C:266:SER:HB2	2.16	0.46
1:A:39:LEU:HD22	1:A:222:ILE:HG23	1.98	0.46
1:A:49:VAL:HG12	1:A:55:PRO:HA	1.97	0.46
1:A:307:GLN:HE22	2:B:441:ARG:HH11	1.63	0.46
2:B:306:ASP:HB2	1:C:241:VAL:HG21	1.97	0.46
1:C:372:ASP:OD1	1:C:374:LEU:N	2.49	0.46
2:B:337:PHE:CD1	2:B:337:PHE:C	2.90	0.45
2:B:256:MET:HE1	2:B:435:LEU:HD21	1.99	0.45
1:C:135:LEU:HD22	1:C:136:PHE:CE1	2.51	0.45
1:A:79:LEU:O	1:A:83:ILE:CD1	2.65	0.45
1:C:108:LEU:HD12	1:C:111:LEU:HB3	1.99	0.45
1:C:252:ASP:HB2	1:C:461:LEU:HD13	1.99	0.45
1:C:297:MET:HE3	1:C:350:GLU:HG3	1.98	0.45
1:A:340:LEU:H	1:A:340:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:HD11	1:A:436:TYR:CE2	2.52	0.45
2:B:342:MET:O	2:B:346:VAL:HG23	2.17	0.45
2:B:360:VAL:O	2:B:361:LEU:HD12	2.16	0.45
1:C:89:ALA:CB	1:C:122:VAL:HG21	2.42	0.45
1:A:292:ARG:NE	1:A:294:GLU:OE2	2.47	0.45
2:B:131:THR:HG22	2:B:131:THR:O	2.17	0.45
1:C:72:VAL:HG21	1:C:77:PHE:CD2	2.52	0.45
1:C:364:ILE:HD11	1:C:380:LEU:CD1	2.46	0.45
1:A:64:ARG:NH2	1:A:66:GLU:OE2	2.50	0.45
1:A:423:LEU:HD11	1:A:436:TYR:HE2	1.81	0.45
2:B:332:ALA:HB1	1:C:237:LEU:HB3	1.98	0.45
2:B:223:ASP:OD1	2:B:223:ASP:N	2.47	0.45
2:B:235:LEU:O	2:B:389:ASN:ND2	2.44	0.45
2:B:64:ARG:HG2	2:B:67:ASP:OD1	2.16	0.44
1:C:62:GLU:CD	1:C:131:THR:HG21	2.37	0.44
1:A:338:TYR:O	1:A:342:MET:HB2	2.17	0.44
1:C:79:LEU:O	1:C:83:ILE:HG13	2.18	0.44
1:A:150:ARG:O	1:A:154:ASP:CG	2.56	0.44
2:B:297:MET:HE2	2:B:299:PHE:CE2	2.53	0.44
2:B:297:MET:HG3	2:B:354:PHE:CD2	2.53	0.44
1:C:150:ARG:HA	1:C:150:ARG:HD3	1.70	0.44
1:A:348:LEU:CD1	1:A:386:PHE:CG	3.01	0.44
1:A:420:VAL:CG1	1:A:435:LEU:HD11	2.48	0.44
1:C:7:PRO:HG2	1:C:52:HIS:CE1	2.52	0.44
2:B:297:MET:HG2	2:B:329:ARG:HB3	1.99	0.43
1:A:348:LEU:O	1:A:352:MET:HG3	2.18	0.43
1:C:338:TYR:O	1:C:343:HIS:ND1	2.50	0.43
2:B:72:VAL:HG21	2:B:79:LEU:HD12	1.99	0.43
2:B:335:PRO:HA	2:B:343:HIS:NE2	2.33	0.43
1:C:436:TYR:CE1	1:C:449:VAL:HG13	2.52	0.43
1:A:29:VAL:HG21	1:A:40:PHE:CD2	2.52	0.43
1:A:56:GLY:O	1:A:88:ILE:HA	2.19	0.43
1:C:208:TYR:HB3	1:C:213:HIS:CE1	2.54	0.43
1:C:75:LEU:HB3	1:C:77:PHE:CE1	2.54	0.43
1:C:178:GLY:O	1:C:179:LEU:HD12	2.19	0.43
1:A:245:ARG:CZ	1:A:258:ALA:O	2.67	0.43
1:C:380:LEU:HD23	1:C:412:LEU:HD21	2.01	0.43
2:B:437:LEU:HD23	2:B:445:HIS:HB2	2.00	0.43
1:A:253:LEU:HD13	1:A:435:LEU:HD21	1.99	0.43
1:A:45:LEU:CD1	1:A:128:VAL:HG23	2.45	0.43
2:B:68:ILE:O	2:B:72:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HD13	1:A:77:PHE:HB3	2.01	0.42
1:A:59:VAL:HG21	1:A:115:LEU:HD23	2.01	0.42
2:B:79:LEU:C	2:B:83:ILE:HD12	2.39	0.42
2:B:246:ILE:CD1	2:B:292:ARG:HH22	2.31	0.42
1:A:58:PHE:CE2	1:A:128:VAL:HG11	2.55	0.42
1:A:129:LEU:HD13	1:A:132:ILE:HD11	2.01	0.42
2:B:435:LEU:HD23	2:B:435:LEU:C	2.38	0.42
1:C:378:SER:CB	1:C:382:ARG:HH21	2.29	0.42
1:C:436:TYR:HE1	1:C:449:VAL:CG1	2.33	0.42
1:A:16:LEU:HD22	1:A:218:TYR:CZ	2.55	0.42
2:B:297:MET:HE2	2:B:299:PHE:CZ	2.54	0.42
1:A:427:VAL:HG23	1:A:427:VAL:O	2.19	0.42
2:B:156:LEU:HD13	2:B:163:THR:HG21	2.01	0.42
1:C:111:LEU:HD21	1:C:115:LEU:HD11	2.01	0.42
1:C:297:MET:CE	1:C:350:GLU:HG3	2.49	0.42
1:C:297:MET:HG3	1:C:356:PRO:HG3	2.02	0.42
1:A:63:GLU:OE1	2:B:209:ARG:NH1	2.53	0.42
1:A:129:LEU:CB	1:A:132:ILE:HD11	2.50	0.41
2:B:79:LEU:HD23	2:B:79:LEU:HA	1.92	0.41
2:B:352:MET:HE3	2:B:386:PHE:CE2	2.55	0.41
1:A:246:ILE:HG22	1:A:264:ARG:HD3	2.02	0.41
1:A:414:SER:O	1:A:441:ARG:NH2	2.54	0.41
2:B:361:LEU:HB3	2:B:364:ILE:HG23	2.02	0.41
1:C:45:LEU:HD13	1:C:128:VAL:HG23	2.03	0.41
1:C:56:GLY:HA2	1:C:126:ARG:O	2.20	0.41
1:C:16:LEU:HD22	1:C:218:TYR:CZ	2.55	0.41
1:A:96:ASP:CG	1:A:97:PRO:HD2	2.41	0.41
2:B:421:LEU:HB3	2:B:436:TYR:HB2	2.02	0.41
1:C:339:SER:N	1:C:342:MET:HB3	2.35	0.41
1:C:372:ASP:OD1	1:C:375:GLU:HG3	2.21	0.41
1:A:235:LEU:HG	1:A:382:ARG:HG2	2.03	0.41
2:B:230:LEU:HD12	2:B:231:PRO:CD	2.42	0.41
2:B:310:ARG:NH1	1:C:242:HIS:O	2.54	0.41
2:B:439:LYS:HZ1	2:B:441:ARG:HH21	1.67	0.41
1:C:246:ILE:HD12	1:C:393:THR:HG21	2.01	0.41
1:A:46:ILE:O	1:A:49:VAL:HG22	2.20	0.41
1:C:39:LEU:CD2	1:C:222:ILE:HG23	2.51	0.41
1:C:230:LEU:C	1:C:230:LEU:HD23	2.41	0.41
1:C:425:ARG:NH1	1:C:434:GLU:OE1	2.54	0.41
1:A:10:ILE:HG22	1:A:13:PHE:H	1.85	0.41
2:B:191:ASP:OD2	2:B:193:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:VAL:HG22	1:A:393:THR:CG2	2.51	0.41
1:A:384:VAL:HG21	1:A:415:LEU:HD21	2.02	0.41
1:C:426:GLU:HB2	1:C:431:PHE:CE2	2.55	0.41
1:A:376:VAL:O	1:A:380:LEU:HG	2.21	0.40
2:B:284:HIS:ND1	2:B:317:LEU:HD11	2.37	0.40
2:B:427:VAL:O	2:B:427:VAL:HG23	2.21	0.40
1:C:12:GLY:HA3	1:C:229:VAL:HB	2.02	0.40
2:B:282:ALA:HB1	2:B:360:VAL:HG13	2.03	0.40
1:C:203:LEU:HD23	1:C:203:LEU:C	2.41	0.40
1:C:221:LEU:HD23	1:C:221:LEU:HA	1.93	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	424/490 (86%)	405 (96%)	18 (4%)	1 (0%)	47 78
1	C	440/490 (90%)	423 (96%)	15 (3%)	2 (0%)	29 61
2	B	432/490 (88%)	416 (96%)	16 (4%)	0	100 100
All	All	1296/1470 (88%)	1244 (96%)	49 (4%)	3 (0%)	47 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	PRO
1	C	96	ASP
1	C	339	SER

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	350/396 (88%)	338 (97%)	12 (3%)	37	71
1	C	361/396 (91%)	345 (96%)	16 (4%)	28	61
2	B	353/395 (89%)	335 (95%)	18 (5%)	24	56
All	All	1064/1187 (90%)	1018 (96%)	46 (4%)	29	62

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	A	86	GLU
1	A	117	LEU
1	A	159	ARG
1	A	161	LEU
1	A	208	TYR
1	A	330	PHE
1	A	342	MET
1	A	348	LEU
1	A	349	ARG
1	A	456	ASP
1	A	457	ARG
2	B	37	LYS
2	B	81	LYS
2	B	179	LEU
2	B	191	ASP
2	B	199	SER
2	B	204	ARG
2	B	208	TYR
2	B	300	SER
2	B	306	ASP
2	B	324	ASP
2	B	329	ARG
2	B	330	PHE
2	B	337	PHE
2	B	338	TYR

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Mol	Chain	Res	Type
2	B	339	SER
2	B	382	ARG
2	B	425	ARG
2	B	457	ARG
1	C	6	SER
1	C	80	ASP
1	C	111	LEU
1	C	208	TYR
1	C	225	ASP
1	C	257	MET
1	C	313	ARG
1	C	321	ARG
1	C	323	ARG
1	C	334	ARG
1	C	339	SER
1	C	343	HIS
1	C	365	SER
1	C	390	ARG
1	C	452	PHE
1	C	460	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	307	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SEP	B	414	2	8,9,10	1.55	1 (12%)	8,12,14	1.81	2 (25%)

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	SEP	B	414	2	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	414	SEP	P-O1P	3.42	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	414	SEP	OG-CB-CA	3.61	111.66	108.14
2	B	414	SEP	P-OG-CB	-2.99	110.05	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	414	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	A	601	-	24,29,29	0.95	2 (8%)	29,45,45	1.50	5 (17%)
3	ADP	C	601	-	24,29,29	0.98	2 (8%)	29,45,45	1.52	5 (17%)
3	ADP	C	602	-	24,29,29	0.96	2 (8%)	29,45,45	1.39	3 (10%)
3	ADP	B	601	-	24,29,29	0.88	1 (4%)	29,45,45	1.52	6 (20%)
3	ADP	A	602	-	24,29,29	0.97	2 (8%)	29,45,45	1.46	3 (10%)
3	ADP	B	602	-	24,29,29	0.96	2 (8%)	29,45,45	1.47	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	601	-	-	4/12/32/32	0/3/3/3
3	ADP	C	601	-	-	3/12/32/32	0/3/3/3
3	ADP	C	602	-	-	6/12/32/32	0/3/3/3
3	ADP	B	601	-	-	1/12/32/32	0/3/3/3
3	ADP	A	602	-	-	7/12/32/32	0/3/3/3
3	ADP	B	602	-	-	3/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ADP	O4'-C1'	2.50	1.44	1.41
3	C	602	ADP	O4'-C1'	2.44	1.44	1.41
3	A	602	ADP	O4'-C1'	2.41	1.44	1.41
3	B	602	ADP	O4'-C1'	2.41	1.44	1.41
3	C	601	ADP	C5-C4	2.24	1.46	1.40
3	B	602	ADP	C5-C4	2.23	1.46	1.40
3	A	601	ADP	C5-C4	2.20	1.46	1.40
3	B	601	ADP	C5-C4	2.18	1.46	1.40
3	A	601	ADP	O4'-C1'	2.16	1.44	1.41
3	A	602	ADP	C5-C4	2.15	1.46	1.40
3	C	602	ADP	C5-C4	2.13	1.46	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601	ADP	C3'-C2'-C1'	3.78	106.67	100.98
3	B	602	ADP	C3'-C2'-C1'	3.75	106.63	100.98
3	B	601	ADP	N3-C2-N1	-3.74	122.84	128.68
3	C	602	ADP	N3-C2-N1	-3.66	122.96	128.68
3	A	602	ADP	N3-C2-N1	-3.64	122.98	128.68
3	B	602	ADP	N3-C2-N1	-3.60	123.06	128.68
3	A	601	ADP	N3-C2-N1	-3.59	123.07	128.68
3	A	602	ADP	C3'-C2'-C1'	3.54	106.31	100.98
3	C	601	ADP	N3-C2-N1	-3.50	123.21	128.68
3	A	602	ADP	PA-O3A-PB	-3.33	121.39	132.83
3	A	601	ADP	C3'-C2'-C1'	3.32	105.98	100.98
3	A	601	ADP	PA-O3A-PB	-3.28	121.58	132.83
3	B	601	ADP	PA-O3A-PB	-3.25	121.68	132.83
3	B	601	ADP	C3'-C2'-C1'	3.18	105.77	100.98
3	C	602	ADP	PA-O3A-PB	-3.15	122.01	132.83
3	C	601	ADP	C4-C5-N7	-3.05	106.22	109.40
3	C	601	ADP	PA-O3A-PB	-2.81	123.17	132.83
3	A	601	ADP	C4-C5-N7	-2.74	106.54	109.40
3	B	602	ADP	PA-O3A-PB	-2.73	123.45	132.83
3	C	602	ADP	C3'-C2'-C1'	2.47	104.69	100.98
3	B	602	ADP	C4-C5-N7	-2.44	106.85	109.40
3	B	601	ADP	C2-N1-C6	2.27	122.64	118.75
3	B	601	ADP	O3B-PB-O2B	2.19	116.01	107.64
3	B	601	ADP	C4-C5-N7	-2.12	107.19	109.40
3	C	601	ADP	C2-N1-C6	2.05	122.26	118.75
3	A	601	ADP	C2-N1-C6	2.02	122.20	118.75
3	B	602	ADP	C2-N1-C6	2.01	122.20	118.75

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	C5'-O5'-PA-O1A
3	A	602	ADP	PA-O3A-PB-O3B
3	A	602	ADP	C5'-O5'-PA-O3A
3	B	602	ADP	C5'-O5'-PA-O1A
3	B	602	ADP	C5'-O5'-PA-O2A
3	C	601	ADP	C5'-O5'-PA-O1A
3	C	601	ADP	C5'-O5'-PA-O2A
3	C	602	ADP	C5'-O5'-PA-O1A
3	C	602	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	A	602	ADP	O4'-C4'-C5'-O5'
3	C	602	ADP	O4'-C4'-C5'-O5'
3	A	602	ADP	C3'-C4'-C5'-O5'
3	C	602	ADP	C3'-C4'-C5'-O5'
3	B	602	ADP	C5'-O5'-PA-O3A
3	C	602	ADP	C5'-O5'-PA-O3A
3	A	601	ADP	C5'-O5'-PA-O2A
3	A	602	ADP	C5'-O5'-PA-O1A
3	A	602	ADP	C5'-O5'-PA-O2A
3	A	601	ADP	C3'-C4'-C5'-O5'
3	C	602	ADP	PB-O3A-PA-O1A
3	A	602	ADP	PA-O3A-PB-O2B
3	A	601	ADP	C5'-O5'-PA-O3A
3	C	601	ADP	C5'-O5'-PA-O3A
3	B	601	ADP	PB-O3A-PA-O1A

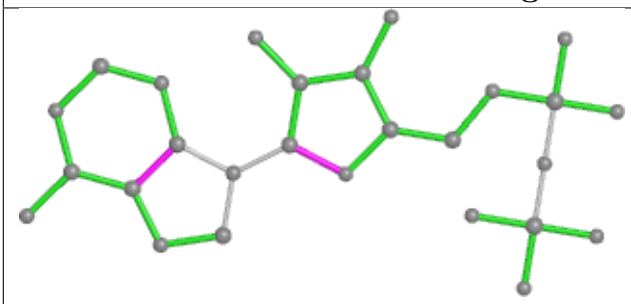
There are no ring outliers.

2 monomers are involved in 2 short contacts:

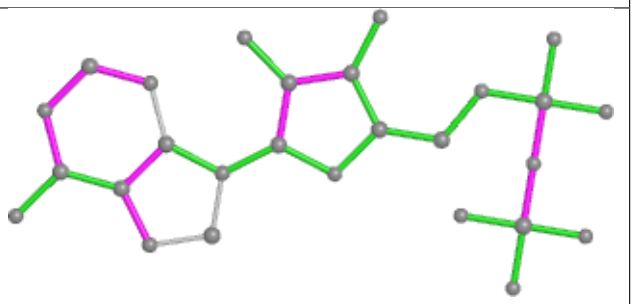
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	1	0
3	C	602	ADP	1	0

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

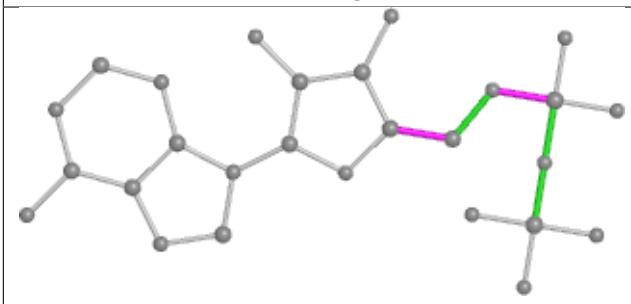
Ligand ADP A 601



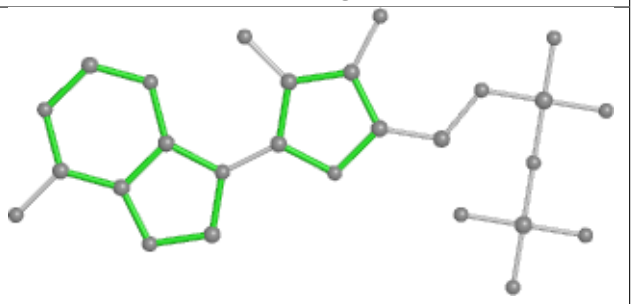
Bond lengths



Bond angles

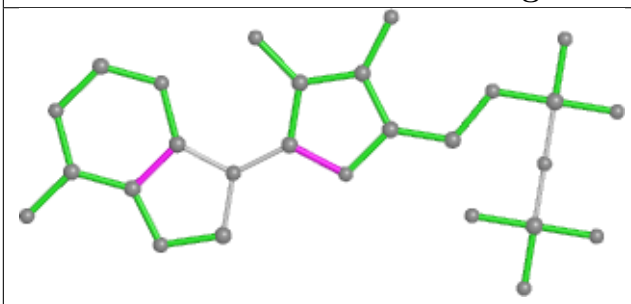


Torsions

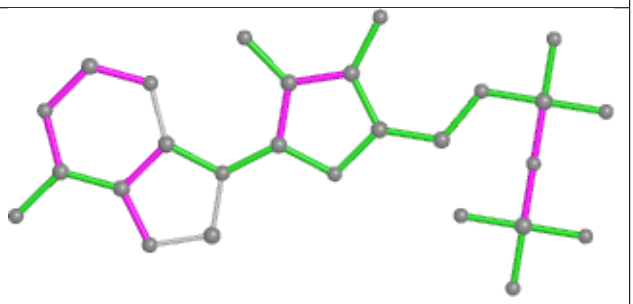


Rings

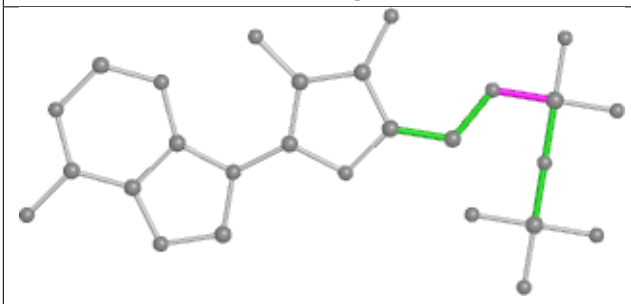
Ligand ADP C 601



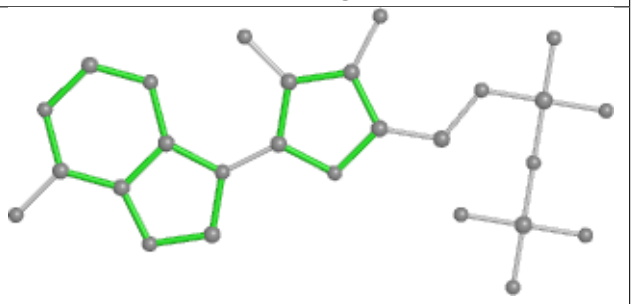
Bond lengths



Bond angles

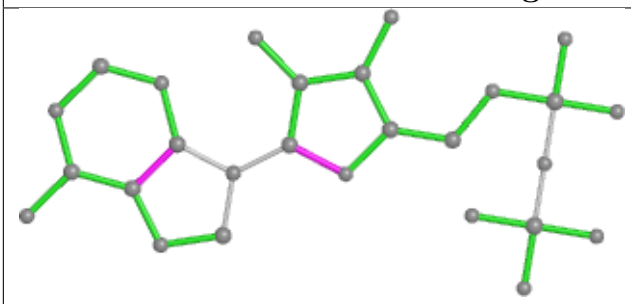


Torsions

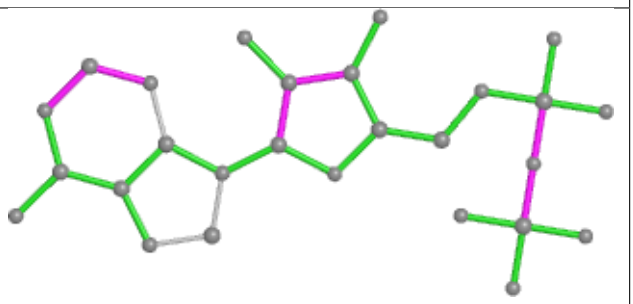


Rings

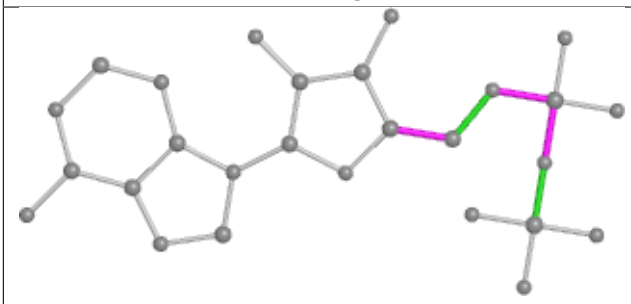
Ligand ADP C 602



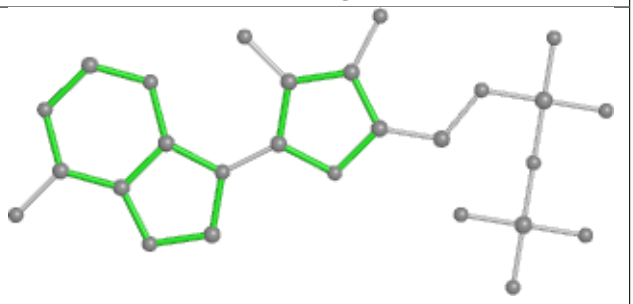
Bond lengths



Bond angles

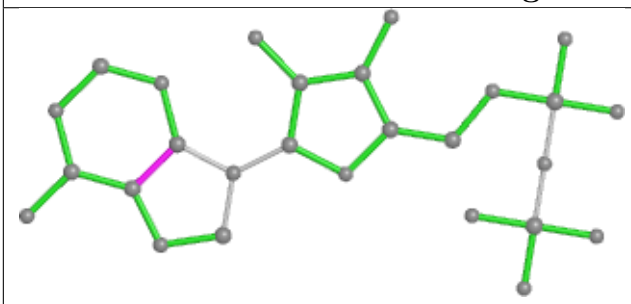


Torsions

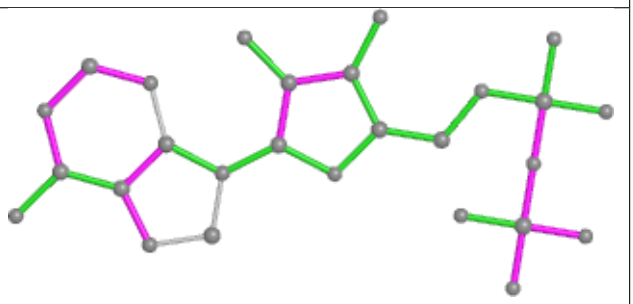


Rings

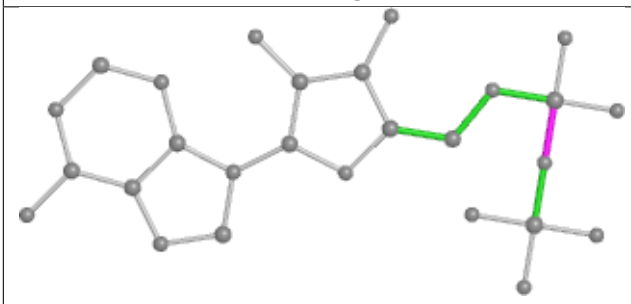
Ligand ADP B 601



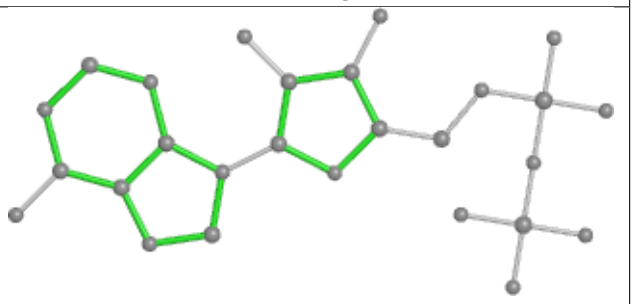
Bond lengths



Bond angles

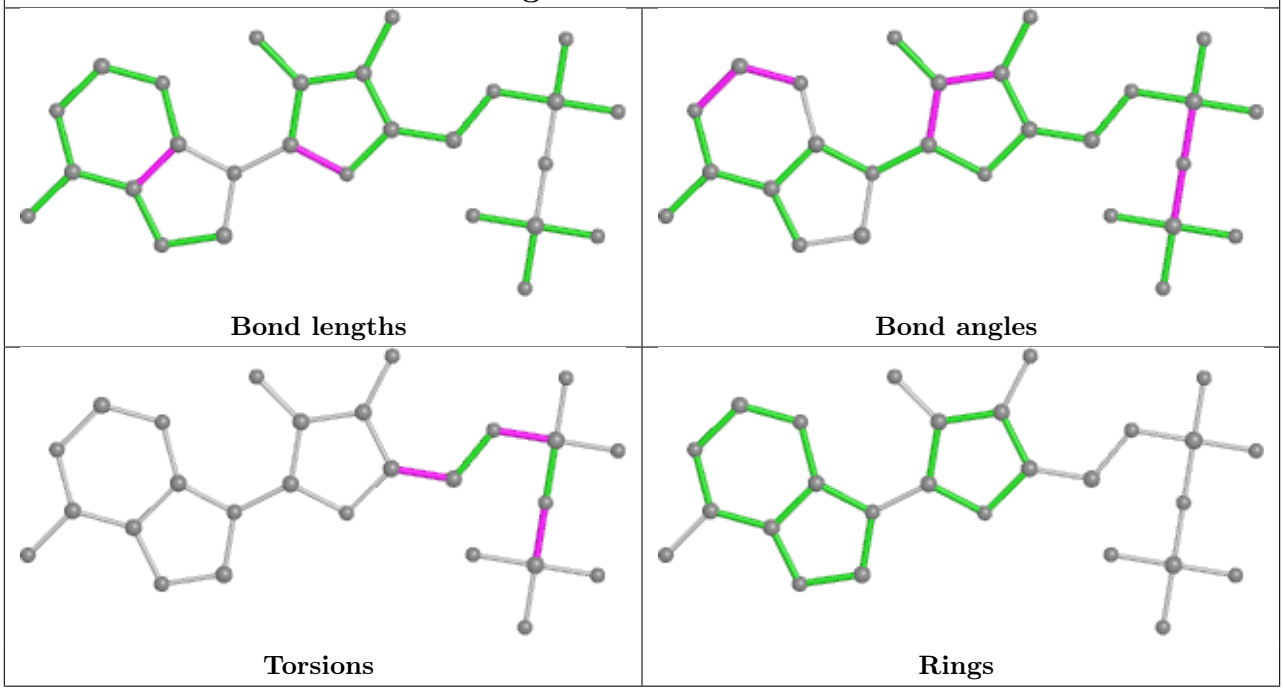


Torsions

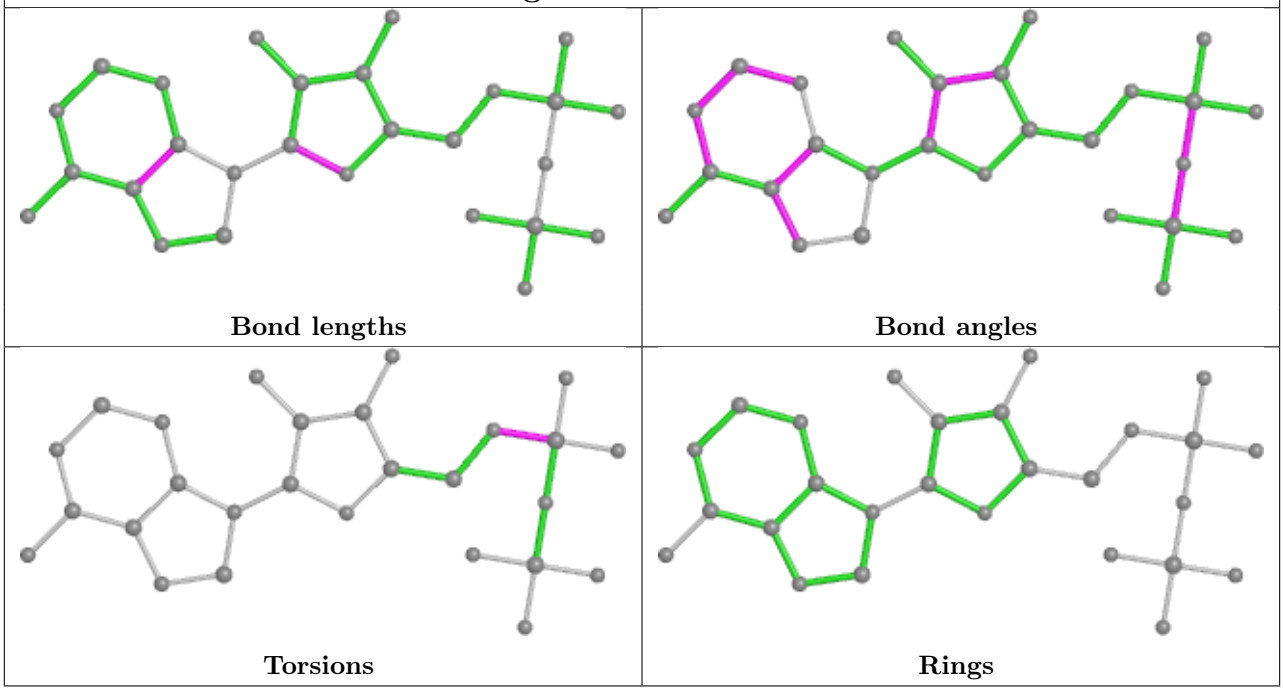


Rings

Ligand ADP A 602



Ligand ADP B 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	434/490 (88%)	0.53	25 (5%)	23	19	28, 54, 93, 122	0
1	C	446/490 (91%)	0.39	11 (2%)	57	55	25, 46, 88, 131	0
2	B	438/490 (89%)	0.32	8 (1%)	68	67	27, 45, 82, 115	0
All	All	1318/1470 (89%)	0.41	44 (3%)	46	41	25, 49, 90, 131	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	447	ASN	4.9
1	C	436	TYR	4.1
1	A	430	GLU	3.7
1	A	95	VAL	3.4
1	A	431	PHE	3.3
1	A	453	LEU	3.3
1	C	99	GLU	3.2
1	A	380	LEU	3.2
1	A	424	ASN	2.9
1	C	337	PHE	2.9
2	B	428	ASN	2.7
1	A	436	TYR	2.6
1	A	412	LEU	2.6
1	A	2	GLY	2.5
2	B	435	LEU	2.5
1	C	108	LEU	2.5
1	C	424	ASN	2.5
1	A	253	LEU	2.5
2	B	436	TYR	2.4
1	A	440	ALA	2.4
1	C	420	VAL	2.3
1	A	437	LEU	2.3
1	A	377	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	273	VAL	2.3
1	A	96	ASP	2.3
1	A	452	PHE	2.3
1	C	111	LEU	2.2
1	C	421	LEU	2.2
2	B	344	LEU	2.2
1	A	87	LYS	2.1
1	A	261	GLY	2.1
1	C	437	LEU	2.1
1	A	90	ILE	2.1
2	B	237	LEU	2.1
1	C	61	PHE	2.1
1	A	111	LEU	2.1
1	A	459	ILE	2.1
2	B	449	VAL	2.0
1	A	112	PHE	2.0
1	C	461	LEU	2.0
1	A	237	LEU	2.0
1	A	421	LEU	2.0
1	A	435	LEU	2.0
2	B	431	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	SEP	B	414	10/11	0.77	0.34	91,100,116,116	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

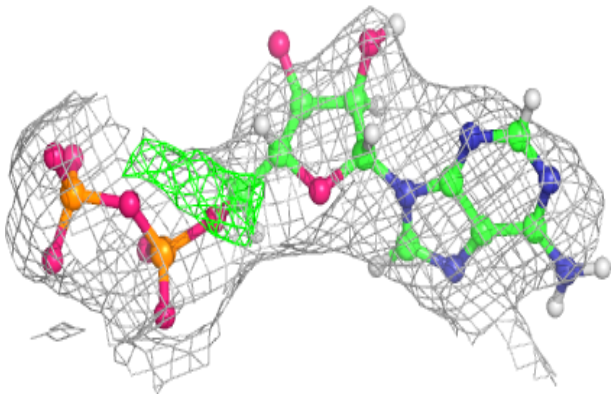
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

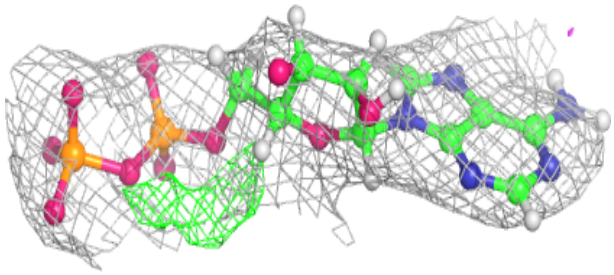
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	A	601	27/27	0.93	0.21	46,51,65,68	0
3	ADP	C	601	27/27	0.94	0.17	35,47,60,62	0
3	ADP	B	601	27/27	0.95	0.18	27,33,43,47	0
3	ADP	B	602	27/27	0.95	0.18	29,42,53,55	0
3	ADP	A	602	27/27	0.95	0.21	32,39,54,59	0
3	ADP	C	602	27/27	0.96	0.18	30,36,49,50	0

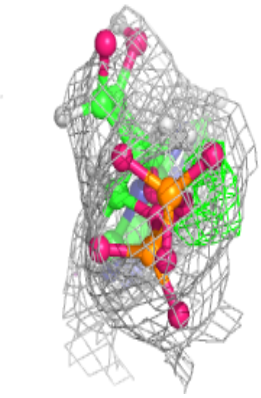
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 601:

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

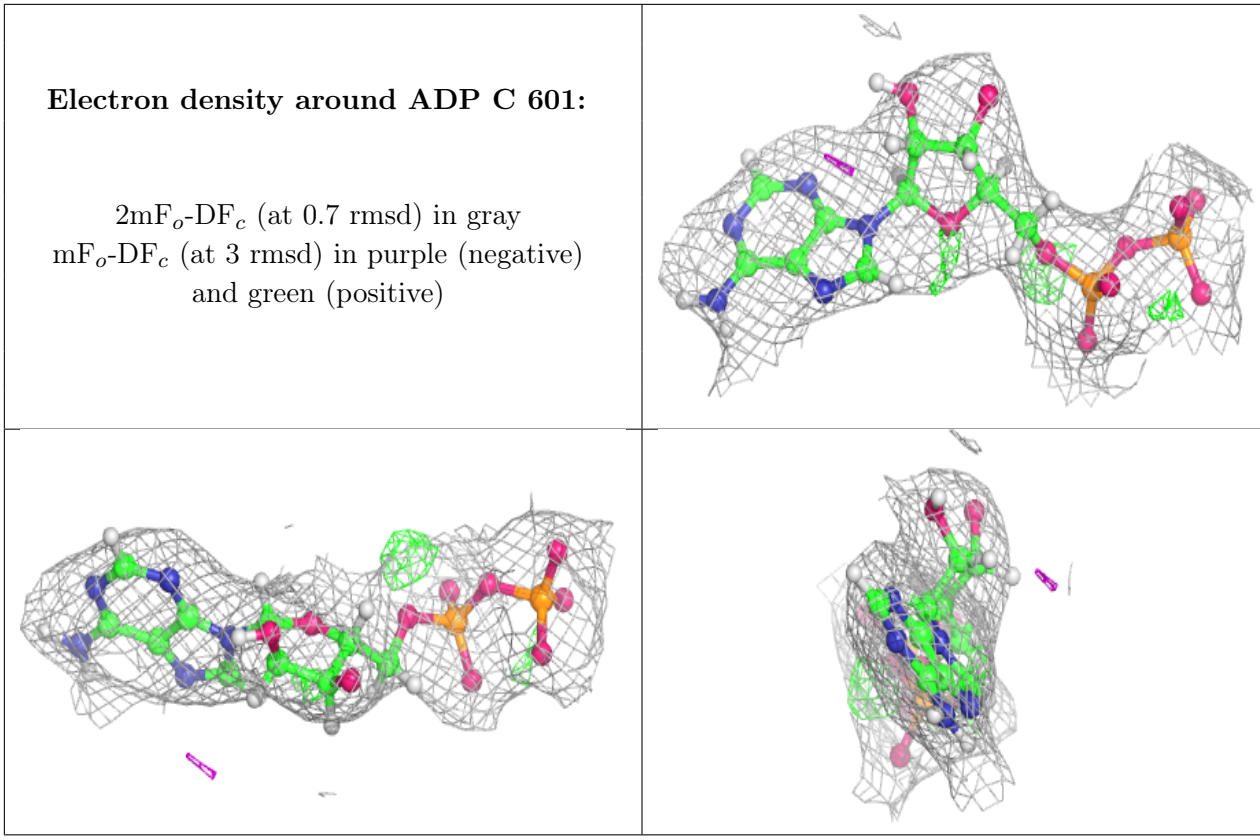






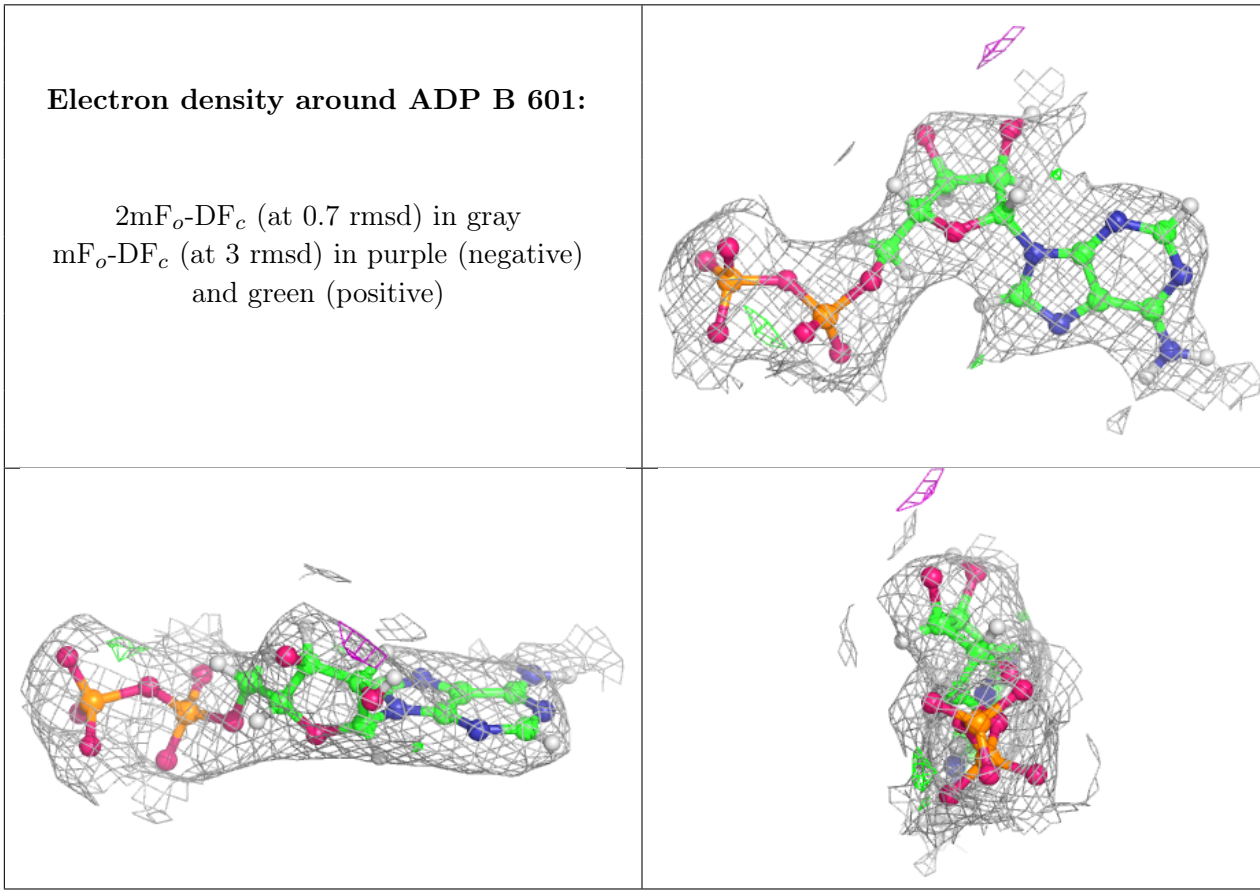
Electron density around ADP C 601:

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



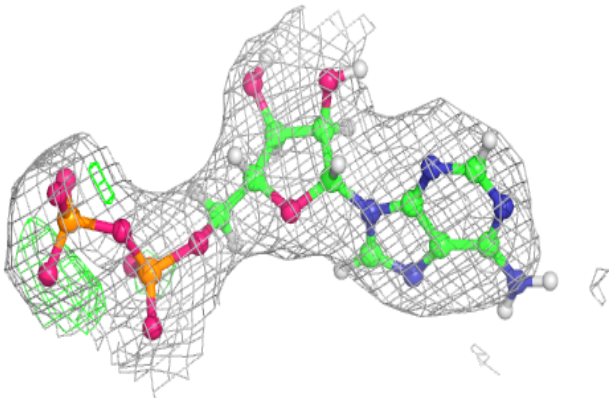
Electron density around ADP B 601:

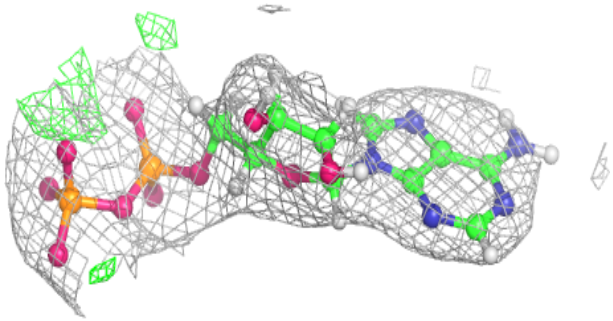
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

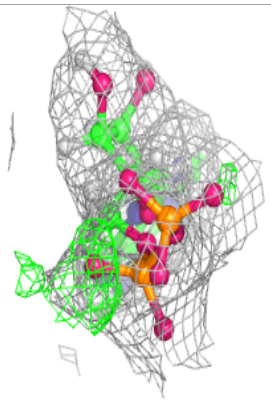


Electron density around ADP B 602:

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

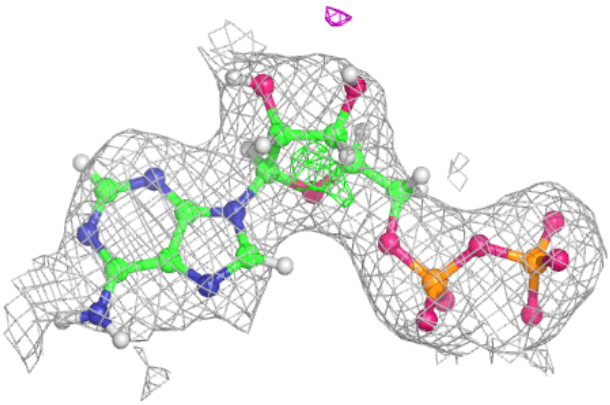


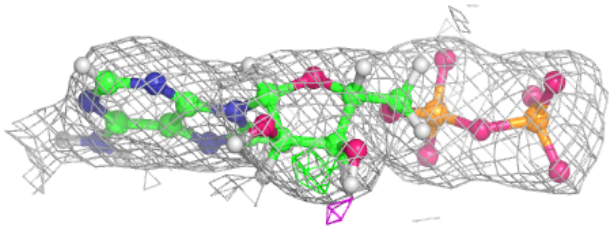


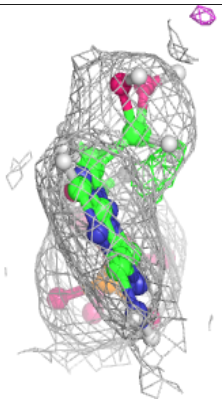


Electron density around ADP A 602:

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

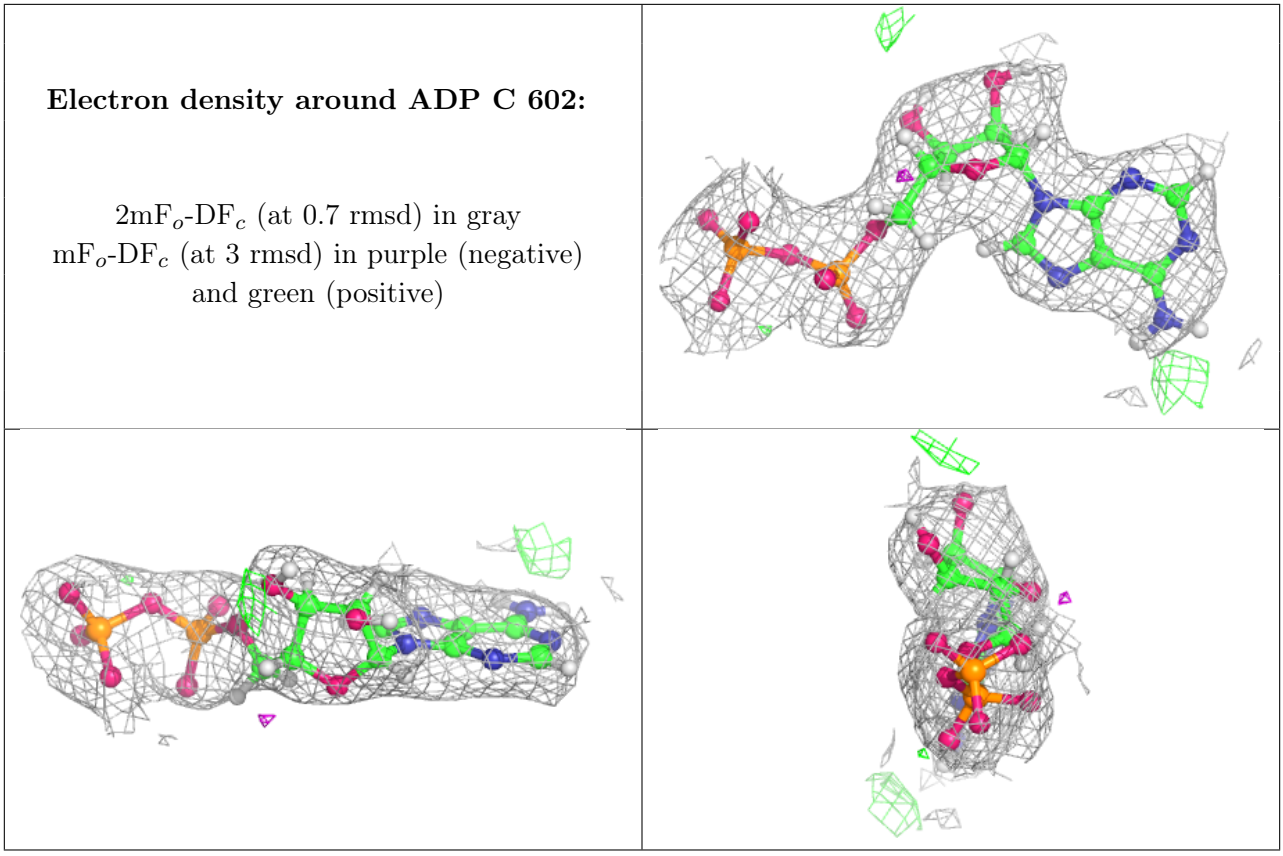






Electron density around ADP C 602:

$2mF_o$-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.