Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 05:02 PM EDT

PDB ID	:	5FHH
Title	:	Structure of human Pif1 helicase domain residues 200-641
Authors	:	Zhou, X.; Ren, W.; Bharath, S.R.; Song, H.
Deposited on	:	2015-12-22
Resolution	:	3.60 Å(reported)

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

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

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

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

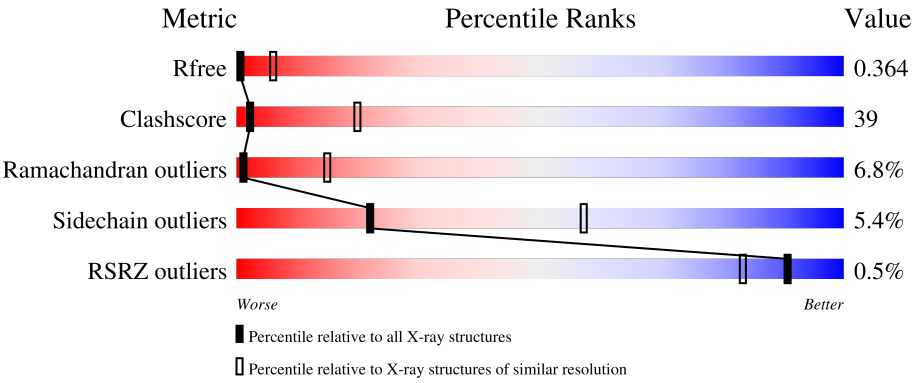
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	442	43% 40% 6% 11%
1	B	442	% 48% 36% · 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ALF	A	702	-	-	X	-
3	ALF	B	702	-	-	X	-

2 Entry composition (i)

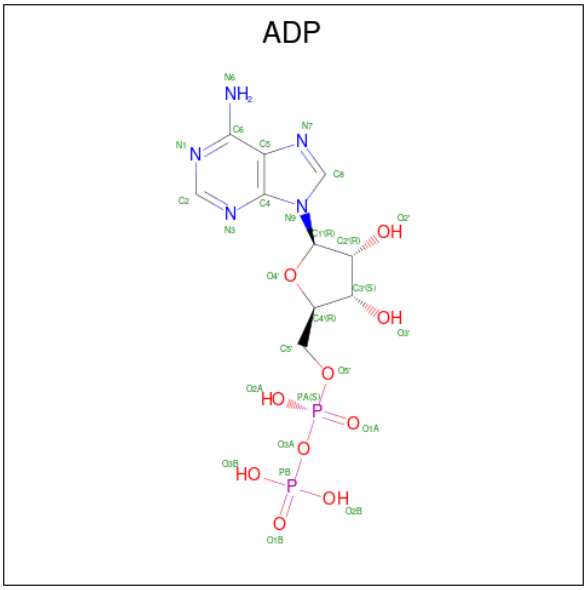
There are 3 unique types of molecules in this entry. The entry contains 5128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent DNA helicase PIF1.

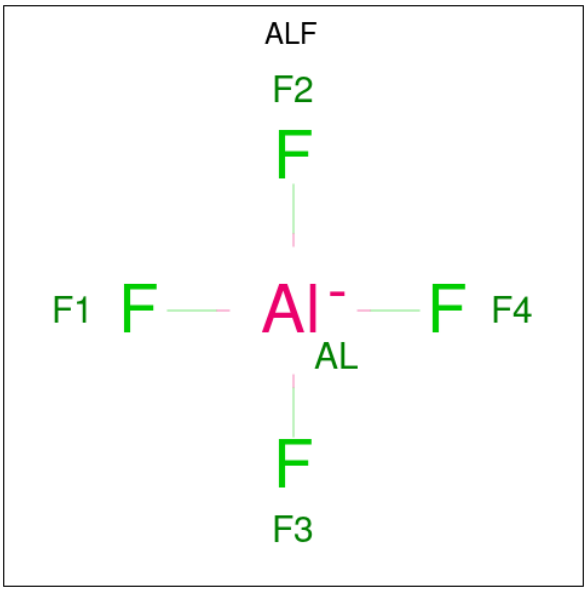
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2622	1656	470	482	14			
1	B	393	Total	C	N	O	S	0	0	0
			2442	1536	430	465	11			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



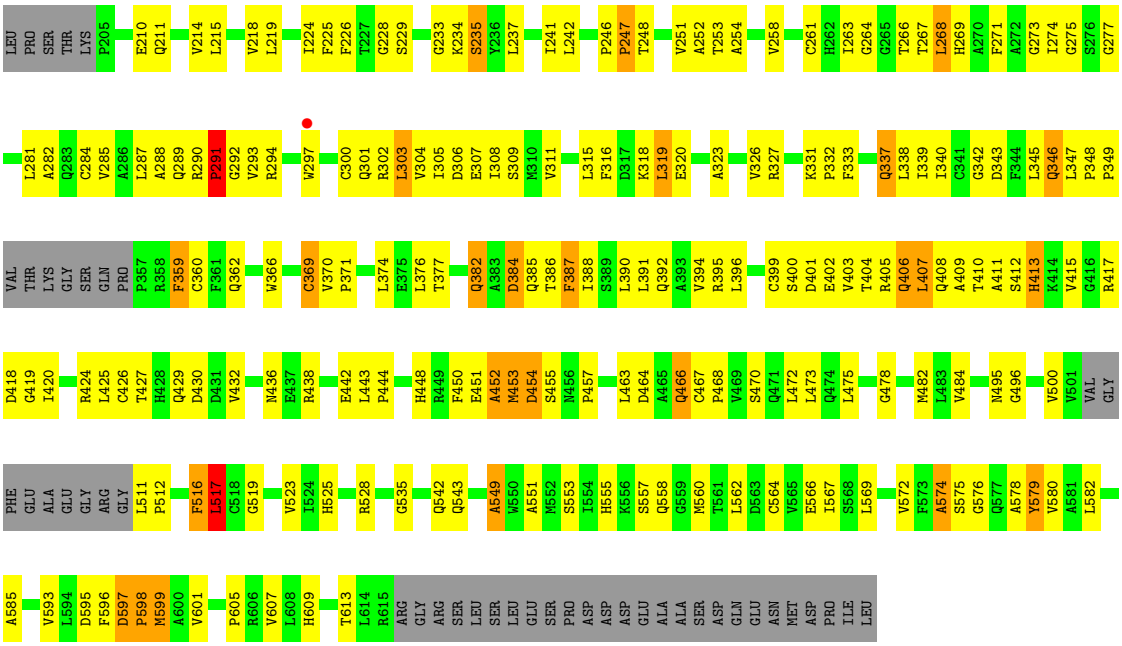
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Al F 5 1 4	0	0
3	B	1	Total Al F 5 1 4	0	0

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.

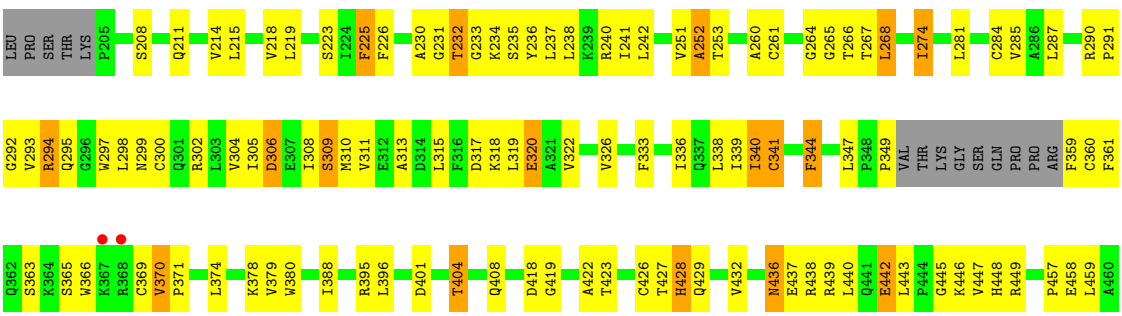
• Molecule 1: ATP-dependent DNA helicase PIF1

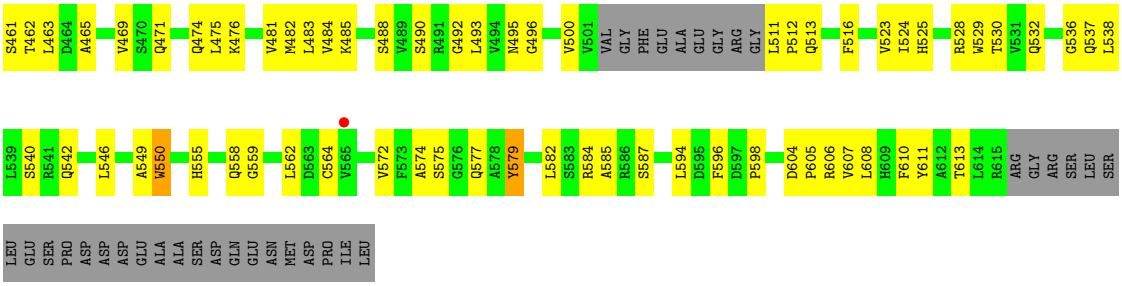
Chain A:



• Molecule 1: ATP-dependent DNA helicase PIF1

Chain B:




S461 T462 L463 D464 A465
V469 S470 Q471
Q474 L475 K476
V481 M482 L483 V484 K485
S488 V489 S490 R491 G492 L493 V494 N495 G496
V500 V501 VAL GLY PHE GLU ALA GLU GLY ARG GLY L511 P512 Q513
F516
V523 I524 H525
R528 W529 T530 V531 Q532
G536 Q537 L538
L539 S540 R541 Q542
L546
A549 W550
H555
Q558 G559
L562 D563 C564 V565
V572 F573 A574 S575 G576 Q577 A578 Y579
L582 S583 R584 A585 R586 S587
L594 D595 F596 D597 P598
D604 P605 R606 V607 L608
H609 F610 Y611
A612 T613
L614 R615
ARG GLY ARG SER LEU SER
LEU GLU SER PRO ASP ASP ASP GLU ALA ALA SER ASP GLN GLU ASN MET ASP PRO ILE LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	204.75Å 204.75Å 77.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.06 – 3.60 47.06 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.06-3.60) 94.3 (47.06-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.310 , 0.355 0.321 , 0.364	Depositor DCC
R_{free} test set	1043 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	76.6	Xtriage
Anisotropy	1.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 117.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	5128	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: ADP, ALF

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	0.36	0/2669	0.70	2/3661 (0.1%)
1	B	0.34	0/2485	0.68	3/3434 (0.1%)
All	All	0.35	0/5154	0.69	5/7095 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	341	CYS	CA-CB-SG	6.80	126.24	114.00
1	B	287	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	291	PRO	N-CA-C	5.94	127.55	112.10
1	A	235	SER	N-CA-CB	-5.81	101.78	110.50
1	B	287	LEU	CB-CG-CD1	5.73	120.74	111.00

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	2622	0	2314	206	0
1	B	2442	0	1983	166	0
2	A	27	0	12	6	0
2	B	27	0	12	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	3	0
3	B	5	0	0	7	0
All	All	5128	0	4321	370	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 39.

All (370) 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:297:TRP:CZ2	1:A:323:ALA:HA	1.54	1.41
1:B:378:LYS:O	1:B:380:TRP:CD1	1.76	1.38
1:A:297:TRP:HZ2	1:A:323:ALA:CA	1.37	1.36
1:A:290:ARG:CG	1:A:291:PRO:HD2	1.59	1.29
1:A:290:ARG:HG2	1:A:291:PRO:CD	1.67	1.25
1:A:297:TRP:HZ2	1:A:323:ALA:CB	1.49	1.24
1:B:423:THR:HG23	1:B:549:ALA:O	1.05	1.20
1:B:423:THR:CG2	1:B:549:ALA:O	1.95	1.12
1:B:333:PHE:HE2	1:B:336:ILE:HG21	1.13	1.10
1:A:297:TRP:CZ2	1:A:323:ALA:CB	2.34	1.09
1:A:297:TRP:CZ2	1:A:323:ALA:CA	2.21	1.06
1:A:407:LEU:HD23	1:A:407:LEU:H	1.20	1.05
1:A:297:TRP:CE2	1:A:323:ALA:HA	1.92	1.04
1:B:333:PHE:CE2	1:B:336:ILE:CG2	2.40	1.03
1:B:333:PHE:HE2	1:B:336:ILE:CG2	1.72	1.02
1:B:333:PHE:CD2	1:B:336:ILE:HG22	1.93	1.02
1:B:333:PHE:CE2	1:B:336:ILE:HG21	1.95	1.01
1:B:378:LYS:O	1:B:380:TRP:NE1	2.03	0.90
1:A:297:TRP:CZ2	1:A:323:ALA:HB2	2.07	0.87
1:B:378:LYS:O	1:B:380:TRP:HD1	1.50	0.87
1:B:233:GLY:O	1:B:235:SER:N	2.08	0.86
1:A:246:PRO:O	1:A:247:PRO:O	1.95	0.85
1:A:407:LEU:O	1:A:410:THR:N	2.10	0.85
1:A:346:GLN:NE2	3:A:702:ALF:F1	2.00	0.84
1:B:333:PHE:HD2	1:B:336:ILE:HG22	1.41	0.83
1:A:517:LEU:C	1:A:519:GLY:H	1.84	0.81
1:B:333:PHE:CE2	1:B:336:ILE:HG22	2.13	0.80
1:A:229:SER:HA	1:A:395:ARG:NH1	1.98	0.79
1:B:235:SER:OG	2:B:701:ADP:H5'2	1.84	0.78
2:B:701:ADP:O1A	3:B:702:ALF:F3	1.90	0.78
1:A:297:TRP:HD1	1:A:326:VAL:CG1	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:ADP:O3B	3:B:702:ALF:F1	1.94	0.76
1:A:412:SER:O	1:A:413:HIS:O	2.04	0.76
1:B:436:ASN:O	1:B:438:ARG:N	2.20	0.75
1:A:569:LEU:O	1:A:595:ASP:HB3	1.86	0.75
1:A:228:GLY:N	1:A:234:LYS:HD3	2.02	0.75
1:A:528:ARG:HD2	1:B:292:GLY:HA2	1.69	0.75
1:A:574:ALA:O	1:A:576:GLY:N	2.20	0.74
1:B:238:LEU:O	1:B:242:LEU:N	2.17	0.74
1:A:297:TRP:CD1	1:A:326:VAL:HB	2.22	0.74
1:B:320:GLU:HG2	1:B:333:PHE:HA	1.67	0.74
1:A:453:MET:O	1:A:455:SER:N	2.21	0.74
1:B:294:ARG:O	1:B:298:LEU:N	2.20	0.74
1:B:426:CYS:HB2	1:B:432:VAL:HG12	1.68	0.73
1:B:305:ILE:O	1:B:340:ILE:HA	1.89	0.73
1:B:231:GLY:O	1:B:233:GLY:N	2.22	0.72
1:B:482:MET:HA	1:B:495:ASN:HA	1.71	0.72
1:A:401:ASP:O	1:A:405:ARG:N	2.15	0.72
1:A:407:LEU:H	1:A:407:LEU:CD2	2.01	0.72
1:A:420:ILE:HD12	1:A:496:GLY:HA2	1.72	0.71
1:A:392:GLN:HA	1:A:395:ARG:HB3	1.72	0.71
1:A:410:THR:O	1:A:412:SER:N	2.23	0.71
1:A:597:ASP:O	1:A:599:MET:N	2.23	0.71
1:A:320:GLU:HA	1:A:333:PHE:HE1	1.56	0.71
1:A:407:LEU:HD23	1:A:407:LEU:N	2.03	0.70
1:A:277:GLY:O	1:A:318:LYS:NZ	2.23	0.70
1:A:331:LYS:HB3	1:A:332:PRO:HD2	1.74	0.70
1:B:378:LYS:CB	1:B:380:TRP:NE1	2.55	0.69
1:A:297:TRP:HD1	1:A:326:VAL:HG11	1.57	0.69
1:A:253:THR:HG22	1:A:254:ALA:H	1.57	0.69
1:B:445:GLY:O	1:B:447:VAL:N	2.21	0.69
1:B:306:ASP:O	1:B:341:CYS:O	2.11	0.69
1:B:333:PHE:CD2	1:B:333:PHE:O	2.46	0.69
1:B:369:CYS:C	1:B:371:PRO:HD2	2.14	0.69
1:B:308:ILE:O	1:B:310:MET:N	2.27	0.68
1:A:290:ARG:CG	1:A:291:PRO:CD	2.44	0.68
1:A:306:ASP:OD1	1:A:307:GLU:N	2.27	0.68
1:A:425:LEU:HB2	1:A:567:ILE:HG22	1.76	0.67
1:B:233:GLY:O	3:B:702:ALF:F2	2.03	0.67
1:B:260:ALA:O	1:B:264:GLY:N	2.29	0.66
1:A:407:LEU:O	1:A:408:GLN:C	2.28	0.66
1:B:559:GLY:HA2	2:B:701:ADP:O3A	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLY:O	3:B:702:ALF:F3	2.04	0.66
1:A:267:THR:O	1:A:269:HIS:N	2.29	0.66
1:B:429:GLN:O	1:B:432:VAL:HG22	1.95	0.66
1:A:297:TRP:CH2	1:A:323:ALA:HB2	2.31	0.66
1:B:208:SER:HB3	1:B:211:GLN:HG3	1.78	0.65
1:A:229:SER:HA	1:A:395:ARG:HH12	1.58	0.65
1:A:281:LEU:O	1:A:285:VAL:N	2.16	0.65
1:B:379:VAL:HG21	1:B:388:ILE:HG13	1.77	0.65
1:A:598:PRO:O	1:A:599:MET:O	2.14	0.65
1:A:407:LEU:HG	1:A:408:GLN:H	1.61	0.65
1:A:402:GLU:O	1:A:406:GLN:NE2	2.28	0.65
1:A:407:LEU:HB2	1:A:593:VAL:HG11	1.77	0.65
1:A:517:LEU:C	1:A:519:GLY:N	2.48	0.64
1:A:599:MET:O	1:A:601:VAL:N	2.27	0.64
1:B:317:ASP:OD1	1:B:363:SER:HB2	1.98	0.64
1:B:320:GLU:HG2	1:B:333:PHE:CA	2.27	0.64
1:B:318:LYS:O	1:B:322:VAL:HG23	1.98	0.63
1:B:238:LEU:HD12	1:B:306:ASP:OD1	1.98	0.63
1:A:214:VAL:HB	1:A:237:LEU:HD21	1.81	0.63
1:A:392:GLN:N	1:A:392:GLN:OE1	2.31	0.63
1:B:339:ILE:O	1:B:340:ILE:CB	2.46	0.63
1:B:449:ARG:HA	1:B:474:GLN:HA	1.80	0.62
1:A:542:GLN:HB3	1:B:291:PRO:HB2	1.81	0.62
2:B:701:ADP:O4'	3:B:702:ALF:F4	2.07	0.62
1:A:297:TRP:NE1	1:A:323:ALA:HA	2.13	0.62
1:B:379:VAL:HG11	1:B:388:ILE:HG21	1.80	0.62
1:B:231:GLY:O	3:B:702:ALF:F4	2.08	0.62
1:B:295:GLN:O	1:B:299:ASN:N	2.29	0.62
1:A:412:SER:O	1:A:413:HIS:C	2.37	0.62
1:A:391:LEU:O	1:A:395:ARG:N	2.23	0.62
1:A:403:VAL:HA	1:A:406:GLN:HE22	1.63	0.61
1:A:495:ASN:O	1:A:516:PHE:HB3	2.00	0.61
1:A:343:ASP:OD2	1:A:395:ARG:NH1	2.34	0.61
1:A:517:LEU:O	1:A:519:GLY:N	2.33	0.61
1:B:605:PRO:HG2	1:B:607:VAL:HB	1.83	0.60
1:B:395:ARG:HB2	1:B:579:TYR:HE1	1.67	0.60
1:A:426:CYS:HB2	1:A:432:VAL:HG13	1.82	0.60
2:A:701:ADP:O2B	3:A:702:ALF:F4	2.09	0.60
1:B:238:LEU:CD1	1:B:306:ASP:OD1	2.50	0.60
1:A:347:LEU:HG	1:A:580:VAL:HG21	1.85	0.59
1:B:308:ILE:HD12	1:B:344:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ALA:HA	1:A:304:VAL:HG22	1.85	0.59
1:B:579:TYR:O	1:B:582:LEU:N	2.35	0.59
1:B:315:LEU:O	1:B:319:LEU:N	2.32	0.58
1:B:440:LEU:HA	1:B:443:LEU:HD12	1.85	0.58
1:A:274:ILE:HG21	1:A:284:CYS:SG	2.43	0.58
1:B:463:LEU:HD21	1:B:471:GLN:H	1.68	0.58
1:B:559:GLY:HA2	2:B:701:ADP:PA	2.43	0.58
1:B:215:LEU:O	1:B:219:LEU:HD12	2.03	0.58
1:A:470:SER:H	1:A:543:GLN:HE22	1.52	0.58
1:A:246:PRO:O	1:A:247:PRO:C	2.43	0.58
1:B:395:ARG:HH12	1:B:611:TYR:HE2	1.50	0.58
1:A:297:TRP:CD1	1:A:326:VAL:CB	2.87	0.57
1:A:215:LEU:O	1:A:219:LEU:HD13	2.05	0.57
1:B:513:GLN:HA	1:B:523:VAL:HA	1.86	0.57
1:A:291:PRO:HG3	1:B:542:GLN:HB3	1.85	0.57
1:A:360:CYS:SG	1:A:366:TRP:NE1	2.77	0.57
1:A:549:ALA:O	1:A:551:ALA:N	2.30	0.57
1:B:481:VAL:O	1:B:496:GLY:N	2.36	0.57
1:A:400:SER:OG	1:A:403:VAL:HG23	2.04	0.57
1:B:238:LEU:HD13	1:B:304:VAL:CG2	2.35	0.57
1:A:516:PHE:N	1:A:516:PHE:CD2	2.73	0.57
1:B:308:ILE:HG13	1:B:309:SER:H	1.69	0.56
1:A:233:GLY:HA2	2:A:701:ADP:C8	2.41	0.56
1:B:524:ILE:HG12	1:B:546:LEU:HD21	1.86	0.56
1:A:304:VAL:HG12	1:A:339:ILE:HD12	1.88	0.56
1:A:370:VAL:N	1:A:371:PRO:HD3	2.21	0.56
1:A:598:PRO:O	1:A:599:MET:C	2.44	0.56
1:A:235:SER:HB2	2:A:701:ADP:O1A	2.05	0.56
1:A:528:ARG:HD2	1:B:292:GLY:CA	2.36	0.56
1:B:447:VAL:HA	1:B:476:LYS:HA	1.88	0.56
1:A:482:MET:HA	1:A:495:ASN:HA	1.88	0.55
1:B:378:LYS:CB	1:B:380:TRP:CE2	2.89	0.55
1:A:384:ASP:OD1	1:A:386:THR:OG1	2.23	0.55
1:B:235:SER:N	3:B:702:ALF:F3	2.28	0.55
1:A:288:ALA:HA	1:A:293:VAL:HG11	1.89	0.55
1:B:300:CYS:SG	1:B:336:ILE:HD11	2.46	0.55
1:A:297:TRP:CD1	1:A:326:VAL:HG11	2.40	0.55
1:B:226:PHE:O	1:B:341:CYS:HB2	2.06	0.55
1:B:448:HIS:N	1:B:475:LEU:O	2.39	0.55
1:B:347:LEU:HB2	1:B:558:GLN:OE1	2.06	0.55
1:A:246:PRO:C	1:A:247:PRO:O	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ASP:OD2	1:B:419:GLY:N	2.31	0.54
1:A:246:PRO:HG2	1:A:302:ARG:NH2	2.23	0.54
1:A:294:ARG:HH12	1:B:525:HIS:CE1	2.25	0.54
1:A:432:VAL:O	1:A:436:ASN:HB2	2.06	0.54
1:B:308:ILE:C	1:B:310:MET:H	2.11	0.54
1:A:392:GLN:O	1:A:396:LEU:HD12	2.08	0.54
1:B:462:THR:HG23	1:B:463:LEU:N	2.23	0.54
1:B:322:VAL:O	1:B:326:VAL:HG23	2.07	0.54
1:B:484:VAL:HA	1:B:493:LEU:HA	1.90	0.54
1:A:448:HIS:HB3	1:A:475:LEU:O	2.07	0.53
1:A:246:PRO:HG2	1:A:302:ARG:HH22	1.74	0.53
1:A:332:PRO:HB2	1:A:369:CYS:HA	1.91	0.53
1:B:226:PHE:HA	1:B:374:LEU:O	2.08	0.53
1:A:300:CYS:O	1:A:327:ARG:NH1	2.33	0.53
1:B:401:ASP:O	1:B:404:THR:OG1	2.21	0.53
1:A:387:PHE:CE1	1:A:391:LEU:HD21	2.44	0.52
1:A:297:TRP:HD1	1:A:326:VAL:CB	2.22	0.52
1:A:406:GLN:OE1	1:A:407:LEU:CD2	2.58	0.52
1:A:517:LEU:HD12	1:A:517:LEU:H	1.75	0.52
1:B:308:ILE:O	1:B:311:VAL:HG22	2.09	0.52
1:B:378:LYS:CB	1:B:380:TRP:HE1	2.22	0.52
1:A:304:VAL:HA	1:A:339:ILE:HB	1.92	0.52
1:B:218:VAL:HG11	1:B:241:ILE:HD13	1.92	0.52
1:B:320:GLU:HA	1:B:333:PHE:HD1	1.75	0.52
1:A:415:VAL:HG12	1:A:564:CYS:HB2	1.92	0.51
1:B:361:PHE:C	1:B:363:SER:H	2.14	0.51
1:A:228:GLY:O	1:A:234:LYS:NZ	2.43	0.51
1:A:233:GLY:HA2	2:A:701:ADP:H8	1.76	0.51
1:B:610:PHE:O	1:B:613:THR:OG1	2.28	0.51
1:B:261:CYS:SG	1:B:485:LYS:HA	2.50	0.51
1:B:349:PRO:HD3	1:B:359:PHE:CE1	2.46	0.51
1:A:316:PHE:O	1:A:320:GLU:N	2.44	0.51
1:A:343:ASP:OD1	1:A:345:LEU:N	2.41	0.51
1:B:238:LEU:HA	1:B:241:ILE:HB	1.92	0.51
1:A:290:ARG:HG2	1:A:291:PRO:HD2	0.72	0.51
1:B:427:THR:HG23	1:B:428:HIS:ND1	2.25	0.51
1:B:596:PHE:O	1:B:598:PRO:HD3	2.10	0.51
1:A:302:ARG:HA	1:A:337:GLN:O	2.11	0.51
1:A:400:SER:N	1:A:403:VAL:HB	2.26	0.51
1:A:225:PHE:CD2	1:A:366:TRP:HH2	2.29	0.51
1:A:443:LEU:HD12	1:A:444:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:SER:OG	1:B:344:PHE:HA	2.12	0.50
1:A:224:ILE:HD11	1:A:374:LEU:HD22	1.94	0.50
1:A:605:PRO:HG2	1:A:607:VAL:HG12	1.92	0.50
1:A:258:VAL:HA	1:A:261:CYS:SG	2.51	0.50
1:A:407:LEU:HG	1:A:408:GLN:N	2.26	0.50
1:A:320:GLU:HA	1:A:333:PHE:CE1	2.41	0.50
1:B:463:LEU:HD12	1:B:463:LEU:H	1.76	0.50
1:B:562:LEU:O	1:B:585:ALA:HA	2.12	0.50
1:A:382:GLN:NE2	1:A:391:LEU:HD11	2.28	0.49
1:A:406:GLN:HG2	1:A:407:LEU:N	2.27	0.49
1:A:576:GLY:O	1:A:580:VAL:HG23	2.12	0.49
1:B:252:ALA:HA	1:B:304:VAL:HG13	1.94	0.49
1:B:333:PHE:CD2	1:B:336:ILE:CG2	2.69	0.49
1:A:315:LEU:O	1:A:319:LEU:HB2	2.11	0.49
1:B:226:PHE:CE2	1:B:237:LEU:HD23	2.48	0.49
1:B:422:ALA:HA	1:B:564:CYS:SG	2.53	0.49
1:A:429:GLN:OE1	1:A:432:VAL:HG23	2.12	0.49
1:B:293:VAL:CG1	1:B:297:TRP:HD1	2.26	0.49
1:A:427:THR:HG23	1:A:572:VAL:HG23	1.94	0.49
1:A:598:PRO:C	1:A:599:MET:O	2.49	0.48
1:B:366:TRP:HA	1:B:369:CYS:O	2.13	0.48
1:B:427:THR:HB	1:B:572:VAL:HG12	1.95	0.48
1:B:333:PHE:O	1:B:333:PHE:CG	2.65	0.48
1:A:424:ARG:O	1:A:551:ALA:HA	2.14	0.48
1:A:450:PHE:HD1	1:A:451:GLU:O	1.97	0.48
1:B:223:SER:OG	1:B:338:LEU:N	2.40	0.48
1:B:292:GLY:HA3	1:B:536:GLY:HA2	1.95	0.48
1:A:450:PHE:CD1	1:A:451:GLU:O	2.67	0.48
1:B:344:PHE:CE2	1:B:361:PHE:CD2	3.02	0.47
1:A:228:GLY:CA	1:A:234:LYS:HD3	2.43	0.47
1:A:253:THR:HG21	1:A:268:LEU:HD23	1.97	0.47
1:A:582:LEU:HD12	1:A:582:LEU:H	1.78	0.47
1:A:395:ARG:HD2	1:A:579:TYR:CE2	2.50	0.47
1:A:609:HIS:O	1:A:613:THR:HG23	2.14	0.47
1:A:251:VAL:HG11	1:A:271:PHE:CE1	2.49	0.47
1:B:359:PHE:HD1	1:B:360:CYS:N	2.12	0.47
1:B:436:ASN:HA	1:B:550:TRP:CE3	2.50	0.47
1:A:211:GLN:OE1	2:A:701:ADP:N6	2.45	0.47
1:B:236:TYR:HB2	2:B:701:ADP:N7	2.30	0.47
1:A:251:VAL:HG22	1:A:303:LEU:HA	1.96	0.46
1:A:403:VAL:HA	1:A:406:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LEU:O	1:A:409:ALA:N	2.48	0.46
1:B:496:GLY:HA3	1:B:516:PHE:HA	1.98	0.46
1:B:253:THR:HG22	1:B:266:THR:H	1.80	0.46
1:A:424:ARG:HA	1:A:566:GLU:O	2.15	0.46
1:A:569:LEU:HA	1:A:572:VAL:HG12	1.97	0.46
1:B:365:SER:O	1:B:369:CYS:N	2.48	0.46
1:A:297:TRP:CD1	1:A:326:VAL:CG1	2.88	0.46
1:B:359:PHE:HD1	1:B:360:CYS:H	1.63	0.46
1:A:443:LEU:HD21	1:A:478:GLY:H	1.81	0.46
1:A:448:HIS:NE2	1:A:500:VAL:HG11	2.31	0.46
1:A:572:VAL:O	1:A:572:VAL:HG13	2.15	0.46
1:A:311:VAL:HG13	1:A:315:LEU:HD23	1.98	0.46
1:A:452:ALA:C	1:A:454:ASP:H	2.17	0.46
1:A:406:GLN:HG2	1:A:407:LEU:CD2	2.46	0.45
1:A:401:ASP:O	1:A:404:THR:N	2.49	0.45
1:A:253:THR:HG22	1:A:254:ALA:N	2.29	0.45
1:A:432:VAL:HG21	1:A:553:SER:HB3	1.99	0.45
1:A:347:LEU:HD12	1:A:558:GLN:HG3	1.97	0.45
1:A:463:LEU:HA	1:A:467:CYS:SG	2.57	0.45
1:B:238:LEU:HD13	1:B:304:VAL:HG21	1.98	0.45
1:B:293:VAL:O	1:B:295:GLN:N	2.49	0.45
1:B:308:ILE:HD12	1:B:344:PHE:HE1	1.80	0.45
1:A:246:PRO:HG2	1:A:302:ARG:NH1	2.31	0.45
1:A:308:ILE:HG22	1:A:342:GLY:HA3	1.99	0.45
1:A:424:ARG:HG3	1:A:425:LEU:N	2.32	0.45
1:B:347:LEU:HD21	1:B:555:HIS:HA	1.98	0.45
1:B:462:THR:O	1:B:465:ALA:N	2.50	0.45
1:A:252:ALA:HA	1:A:304:VAL:CG2	2.46	0.45
1:A:305:ILE:HB	1:A:340:ILE:HD13	1.98	0.45
1:A:523:VAL:HG13	1:A:525:HIS:HE1	1.81	0.45
1:B:230:ALA:HA	2:B:701:ADP:O3B	2.17	0.45
1:A:470:SER:H	1:A:543:GLN:NE2	2.12	0.45
1:A:390:LEU:O	1:A:394:VAL:HG23	2.16	0.44
1:B:226:PHE:O	1:B:341:CYS:CB	2.65	0.44
1:B:528:ARG:NH1	1:B:530:THR:CG2	2.80	0.44
1:A:226:PHE:CE2	1:A:237:LEU:HD23	2.52	0.44
1:A:385:GLN:HA	1:A:388:ILE:HB	1.99	0.44
1:A:290:ARG:HD2	1:A:535:GLY:O	2.17	0.44
1:A:401:ASP:C	1:A:403:VAL:N	2.70	0.44
1:A:242:LEU:HD21	1:A:304:VAL:HG11	1.98	0.44
1:A:273:GLY:O	1:A:287:LEU:HD22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LEU:O	1:B:240:ARG:N	2.50	0.44
1:B:251:VAL:HG22	1:B:302:ARG:O	2.17	0.44
1:B:347:LEU:CD2	1:B:555:HIS:HA	2.48	0.44
1:B:267:THR:O	1:B:268:LEU:HB3	2.18	0.44
1:B:379:VAL:HG21	1:B:388:ILE:CG1	2.47	0.44
1:B:458:GLU:O	1:B:459:LEU:HD22	2.18	0.44
1:A:304:VAL:HG12	1:A:339:ILE:CD1	2.48	0.44
1:B:308:ILE:C	1:B:310:MET:N	2.70	0.44
1:A:309:SER:OG	1:A:343:ASP:O	2.29	0.44
1:A:402:GLU:C	1:A:406:GLN:HE22	2.20	0.43
1:A:452:ALA:O	1:A:454:ASP:N	2.44	0.43
1:B:395:ARG:NH1	1:B:611:TYR:HE2	2.14	0.43
1:A:274:ILE:HG22	1:A:275:GLY:N	2.33	0.43
1:A:348:PRO:HB2	1:A:349:PRO:HD2	2.01	0.43
1:A:400:SER:H	1:A:403:VAL:HB	1.83	0.43
1:A:415:VAL:CG1	1:A:564:CYS:HB2	2.48	0.43
1:B:260:ALA:HB1	1:B:265:GLY:O	2.18	0.43
1:B:427:THR:C	1:B:428:HIS:HD1	2.21	0.43
1:B:528:ARG:HH12	1:B:530:THR:HG21	1.82	0.43
1:A:228:GLY:C	1:A:234:LYS:NZ	2.72	0.43
1:B:226:PHE:CZ	1:B:238:LEU:HD21	2.53	0.43
1:B:315:LEU:O	1:B:319:LEU:HB2	2.18	0.43
1:B:511:LEU:N	1:B:512:PRO:HD3	2.34	0.43
1:A:263:ILE:HD11	1:A:306:ASP:OD2	2.17	0.43
1:A:557:SER:HA	1:A:560:MET:SD	2.59	0.43
1:A:528:ARG:CD	1:B:292:GLY:HA2	2.45	0.43
1:B:436:ASN:HA	1:B:550:TRP:HE3	1.83	0.43
1:A:246:PRO:HG2	1:A:302:ARG:CZ	2.48	0.43
1:A:333:PHE:CD2	1:A:338:LEU:HD22	2.52	0.43
1:A:451:GLU:CB	1:A:472:LEU:HA	2.47	0.43
1:A:463:LEU:HA	1:A:467:CYS:HG	1.84	0.43
1:B:396:LEU:O	1:B:608:LEU:HD11	2.19	0.43
1:A:294:ARG:NH1	1:B:525:HIS:CE1	2.87	0.43
1:B:281:LEU:O	1:B:285:VAL:HG23	2.19	0.43
1:B:459:LEU:HB3	1:B:461:SER:OG	2.18	0.43
1:A:218:VAL:O	1:A:337:GLN:NE2	2.46	0.43
1:A:301:GLN:O	1:A:337:GLN:N	2.51	0.43
1:A:210:GLU:OE2	1:A:377:THR:OG1	2.32	0.43
1:B:308:ILE:HG12	1:B:341:CYS:O	2.19	0.43
1:A:229:SER:O	1:A:234:LYS:NZ	2.51	0.42
1:A:406:GLN:HG2	1:A:407:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:O	1:A:413:HIS:N	2.47	0.42
1:B:252:ALA:O	1:B:265:GLY:HA3	2.19	0.42
1:B:379:VAL:O	1:B:380:TRP:CG	2.72	0.42
1:B:395:ARG:HB2	1:B:579:TYR:CE1	2.52	0.42
1:B:579:TYR:C	1:B:579:TYR:CD2	2.91	0.42
1:A:224:ILE:HG13	1:A:374:LEU:HD13	2.00	0.42
1:A:408:GLN:OE1	1:A:596:PHE:CB	2.68	0.42
1:B:532:GLN:HA	1:B:537:GLN:CB	2.49	0.42
1:B:359:PHE:CD1	1:B:360:CYS:N	2.88	0.42
1:B:378:LYS:CB	1:B:380:TRP:CZ2	3.02	0.42
1:A:246:PRO:HG2	1:A:302:ARG:HH12	1.85	0.42
1:A:291:PRO:HG2	1:A:292:GLY:H	1.85	0.42
1:A:438:ARG:O	1:A:442:GLU:HG3	2.19	0.42
1:A:511:LEU:N	1:A:512:PRO:HD3	2.35	0.42
1:B:293:VAL:HG12	1:B:297:TRP:HD1	1.85	0.42
1:B:226:PHE:HZ	1:B:238:LEU:HD21	1.83	0.42
1:B:439:ARG:O	1:B:442:GLU:HG3	2.19	0.42
1:B:483:LEU:CB	1:B:546:LEU:HD23	2.50	0.42
1:B:604:ASP:C	1:B:606:ARG:H	2.21	0.42
1:B:404:THR:O	1:B:408:GLN:N	2.29	0.42
1:A:267:THR:HG21	1:A:466:GLN:HA	2.02	0.41
1:A:218:VAL:HG11	1:A:241:ILE:HD13	2.02	0.41
1:A:289:GLN:HG2	1:A:326:VAL:HG22	2.02	0.41
1:A:562:LEU:O	1:A:585:ALA:HA	2.20	0.41
1:B:492:GLY:C	1:B:493:LEU:HD12	2.40	0.41
1:A:210:GLU:HB3	1:A:376:LEU:HD23	2.02	0.41
1:A:473:LEU:HD23	1:A:473:LEU:HA	1.83	0.41
1:B:215:LEU:HD13	1:B:241:ILE:HG12	2.02	0.41
1:A:289:GLN:HA	1:A:294:ARG:CG	2.50	0.41
1:A:463:LEU:HD12	1:A:463:LEU:H	1.86	0.41
1:B:575:SER:C	1:B:577:GLN:H	2.23	0.41
1:A:247:PRO:O	1:A:248:THR:OG1	2.24	0.41
1:A:347:LEU:HB2	1:A:558:GLN:OE1	2.21	0.41
1:A:401:ASP:C	1:A:403:VAL:H	2.24	0.41
1:B:529:TRP:O	1:B:540:SER:HA	2.21	0.41
1:A:281:LEU:O	1:A:285:VAL:HG12	2.20	0.41
1:A:290:ARG:HD2	1:A:535:GLY:C	2.42	0.41
1:A:359:PHE:O	1:A:362:GLN:HG3	2.21	0.41
1:A:418:ASP:HB3	1:A:419:GLY:H	1.56	0.41
2:A:701:ADP:O2B	3:A:702:ALF:F2	2.29	0.41
1:B:214:VAL:HB	1:B:237:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:HG22	1:B:232:THR:O	2.21	0.41
1:B:379:VAL:HG11	1:B:388:ILE:HG12	2.02	0.41
1:B:462:THR:HG23	1:B:463:LEU:H	1.86	0.41
1:A:289:GLN:HA	1:A:294:ARG:HG3	2.03	0.41
1:B:443:LEU:HD13	1:B:476:LYS:CB	2.51	0.41
1:B:274:ILE:HD12	1:B:284:CYS:HB3	2.03	0.40
1:B:370:VAL:N	1:B:371:PRO:HD2	2.35	0.40
1:B:313:ALA:HB2	1:B:359:PHE:O	2.21	0.40
1:A:294:ARG:O	1:A:297:TRP:N	2.54	0.40
1:A:385:GLN:HA	1:A:388:ILE:HD12	2.04	0.40
1:B:225:PHE:HB2	1:B:340:ILE:O	2.21	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	389/442 (88%)	301 (77%)	59 (15%)	29 (8%)	1 12
1	B	387/442 (88%)	297 (77%)	66 (17%)	24 (6%)	1 17
All	All	776/884 (88%)	598 (77%)	125 (16%)	53 (7%)	1 15

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	PRO
1	A	411	ALA
1	A	413	HIS
1	A	417	ARG
1	A	430	ASP
1	A	452	ALA
1	A	454	ASP

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Mol	Chain	Res	Type
1	A	484	VAL
1	A	575	SER
1	A	597	ASP
1	A	599	MET
1	B	232	THR
1	B	309	SER
1	B	340	ILE
1	B	437	GLU
1	B	446	LYS
1	B	469	VAL
1	B	500	VAL
1	B	538	LEU
1	B	574	ALA
1	A	266	THR
1	A	268	LEU
1	A	453	MET
1	A	464	ASP
1	A	549	ALA
1	B	252	ALA
1	B	436	ASN
1	B	488	SER
1	B	490	SER
1	A	346	GLN
1	A	517	LEU
1	A	574	ALA
1	A	578	ALA
1	B	234	LYS
1	B	594	LEU
1	A	337	GLN
1	A	466	GLN
1	A	598	PRO
1	B	268	LEU
1	B	294	ARG
1	B	404	THR
1	A	282	ALA
1	A	291	PRO
1	B	370	VAL
1	B	457	PRO
1	B	584	ARG
1	B	587	SER
1	A	264	GLY
1	A	369	CYS

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Mol	Chain	Res	Type
1	A	468	PRO
1	B	274	ILE
1	B	290	ARG
1	A	457	PRO

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	216/363 (60%)	203 (94%)	13 (6%)	19 54
1	B	175/363 (48%)	167 (95%)	8 (5%)	27 61
All	All	391/726 (54%)	370 (95%)	21 (5%)	22 57

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	319	LEU
1	A	359	PHE
1	A	382	GLN
1	A	384	ASP
1	A	387	PHE
1	A	399	CYS
1	A	406	GLN
1	A	407	LEU
1	A	516	PHE
1	A	517	LEU
1	A	555	HIS
1	A	579	TYR
1	B	225	PHE
1	B	306	ASP
1	B	320	GLU
1	B	344	PHE
1	B	428	HIS
1	B	442	GLU

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Mol	Chain	Res	Type
1	B	550	TRP
1	B	579	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	B	701	-	24,29,29	1.02	2 (8%)	29,45,45	1.77	5 (17%)
3	ALF	A	702	-	0,4,4	-	-	-		
3	ALF	B	702	-	0,4,4	-	-	-		
2	ADP	A	701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)

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	ADP	B	701	-	-	4/12/32/32	0/3/3/3
2	ADP	A	701	-	-	3/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ADP	C5-C4	2.72	1.48	1.40
2	B	701	ADP	O4'-C1'	2.50	1.44	1.41
2	B	701	ADP	C5-C4	2.40	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	ADP	C3'-C2'-C1'	4.56	107.85	100.98
2	B	701	ADP	PA-O3A-PB	-3.91	119.41	132.83
2	A	701	ADP	C3'-C2'-C1'	3.67	106.51	100.98
2	A	701	ADP	PA-O3A-PB	-3.29	121.52	132.83
2	B	701	ADP	C4-C5-N7	-3.07	106.20	109.40
2	B	701	ADP	N3-C2-N1	-2.86	124.21	128.68
2	B	701	ADP	O5'-C5'-C4'	2.82	118.69	108.99
2	A	701	ADP	N3-C2-N1	-2.79	124.31	128.68
2	A	701	ADP	C4-C5-N7	-2.55	106.74	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ADP	C5'-O5'-PA-O1A
2	A	701	ADP	C5'-O5'-PA-O2A
2	B	701	ADP	PB-O3A-PA-O5'
2	B	701	ADP	C5'-O5'-PA-O1A
2	B	701	ADP	C3'-C4'-C5'-O5'
2	A	701	ADP	C5'-O5'-PA-O3A
2	B	701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ADP	8	0

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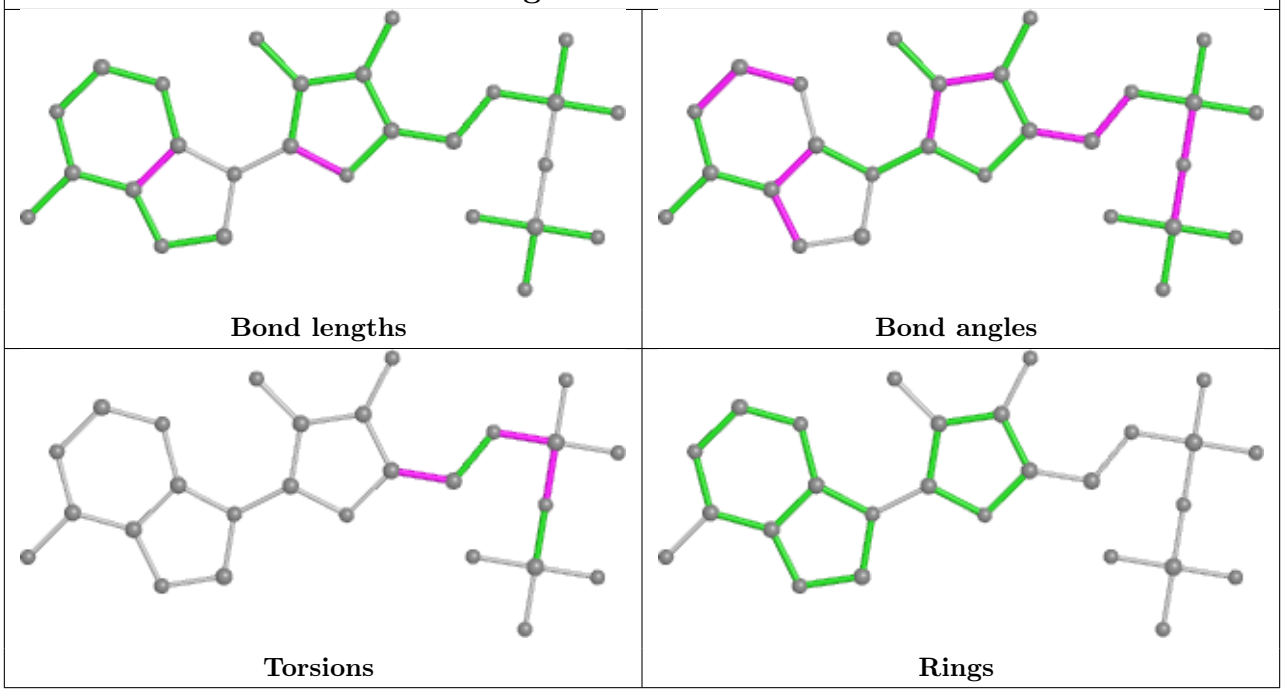
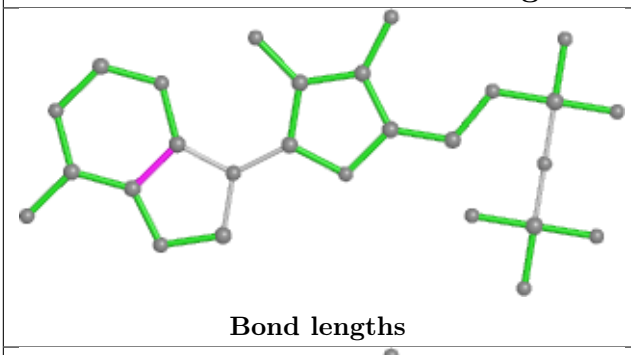
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	ALF	3	0
3	B	702	ALF	7	0
2	A	701	ADP	6	0

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.

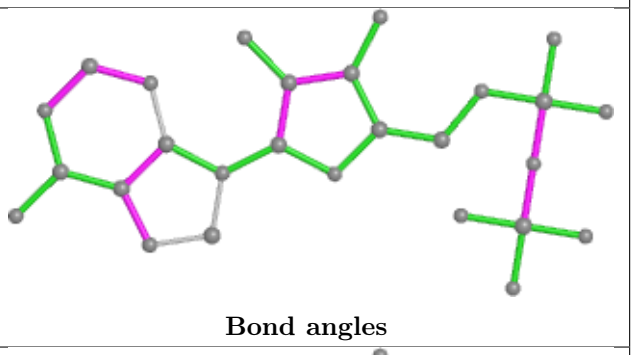
Ligand ADP B 701



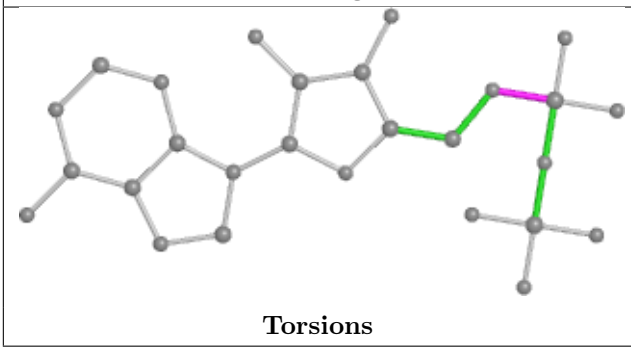
Ligand ADP A 701



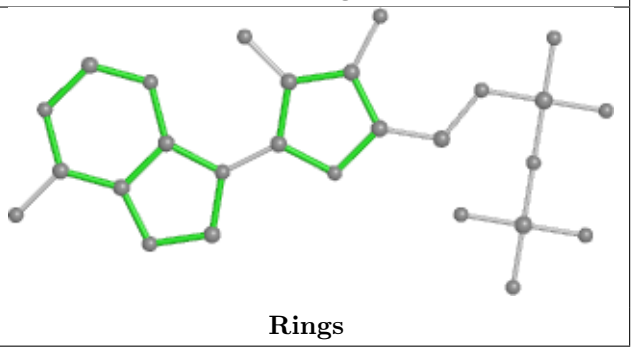
Bond lengths



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	395/442 (89%)	-0.33	1 (0%)	94	88	31, 81, 121, 147	0
1	B	393/442 (88%)	-0.22	3 (0%)	86	75	57, 118, 171, 217	0
All	All	788/884 (89%)	-0.28	4 (0%)	91	83	31, 100, 160, 217	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	LYS	3.3
1	B	368	ARG	3.1
1	B	565	VAL	2.2
1	A	297	TRP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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	ALF	B	702	5/5	0.79	0.18	131,133,139,146	0

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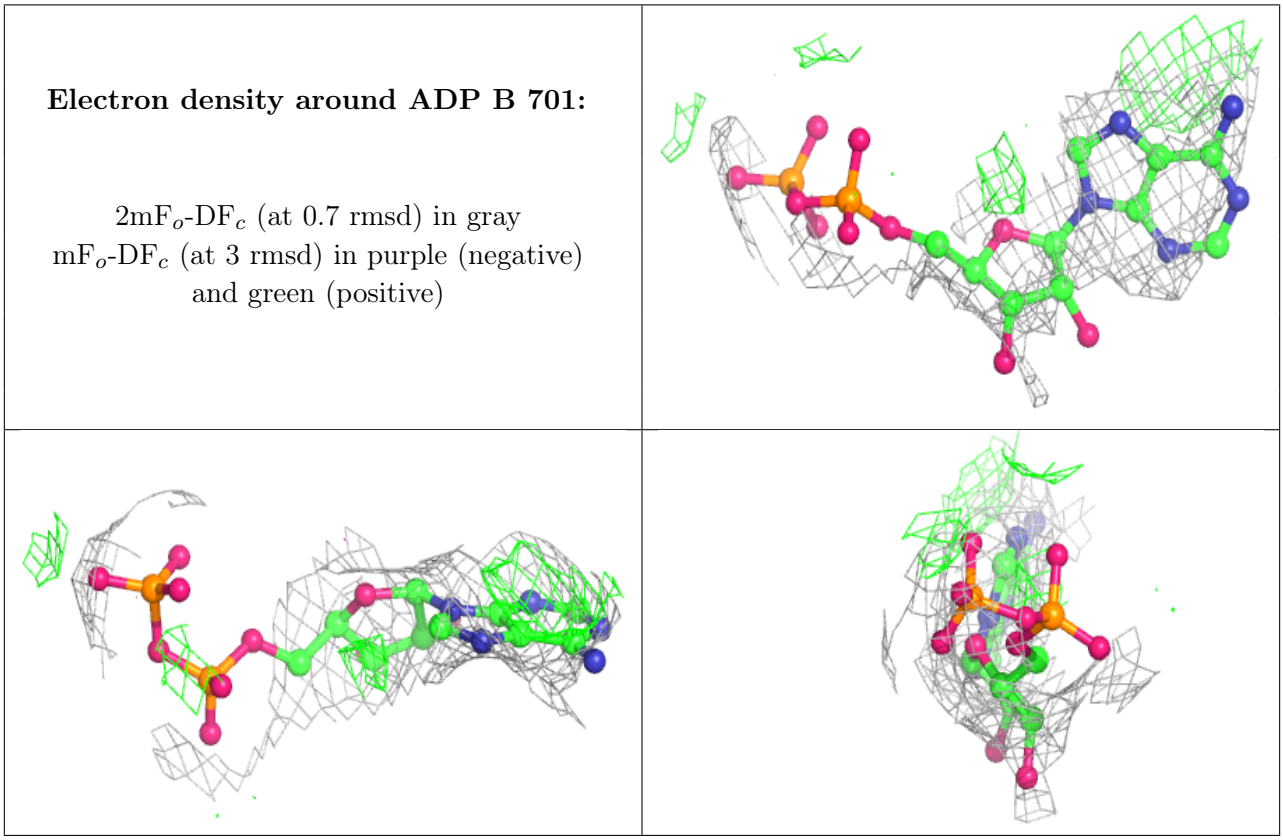
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	B	701	27/27	0.83	0.26	129,150,155,157	0
3	ALF	A	702	5/5	0.87	0.32	91,108,116,118	0
2	ADP	A	701	27/27	0.88	0.30	37,75,114,125	0

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.

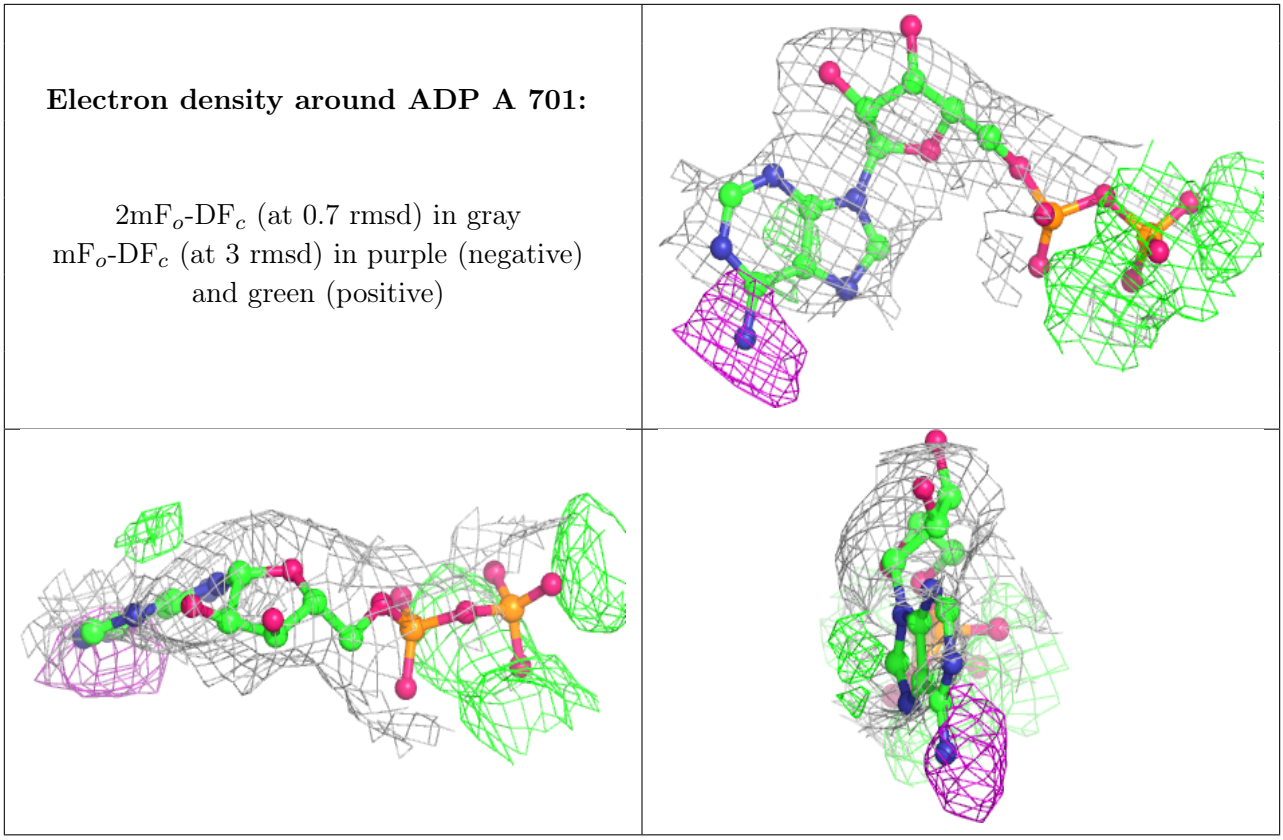
Electron density around ADP B 701:

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



Electron density around ADP A 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.