Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 09:02 AM EST

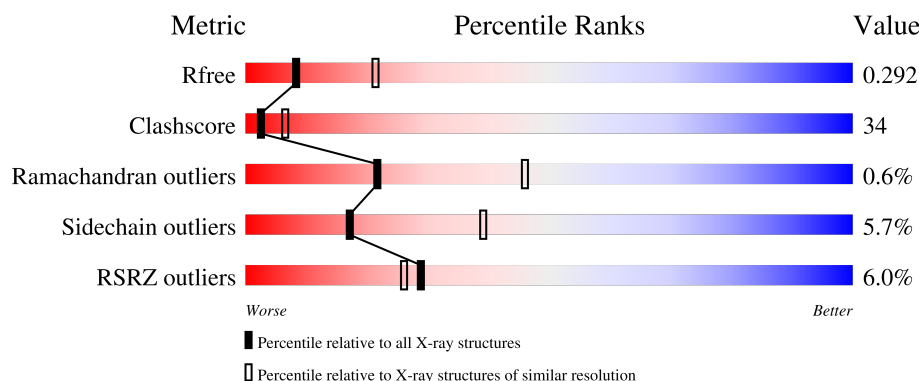|		
PDB ID	:	6MI6
Title	:	STRUCTURE OF CHEA DOMAIN P4 IN COMPLEX WITH AN ADP ANALOG
Authors	:	Crane, B.R.; Muok, A.R.; Chua, T.K.; Le, H.
Deposited on	:	2018-09-19
Resolution	:	2.95 Å(reported)

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1 Overall quality at a glance (i)

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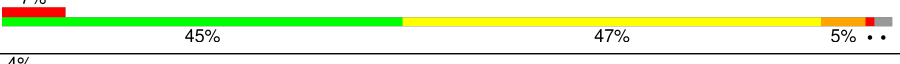*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.292
Clashscore		34
Ramachandran outliers		0.6%
Sidechain outliers		5.7%
RSRZ outliers		6.0%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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%

Mol	Chain	Length	Quality of chain
1	A	187	6% 49% 46% •••
1	B	187	6% 50% 47% ••
1	C	187	7% 45% 47% 5% ••
1	D	187	4% 42% 47% 5% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	601	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5687 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 Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1425	899	249	272	5			
1	B	187	Total	C	N	O	S	0	0	0
			1432	905	246	276	5			
1	C	184	Total	C	N	O	S	0	0	0
			1390	875	239	271	5			
1	D	175	Total	C	N	O	S	0	0	0
			1288	811	223	249	5			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4
O1
O3 — O⁻ — S — O⁻ O4
S
O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total O S 5 4 1			0	0
2	C	1	Total O S 5 4 1			0	0

- Molecule 3 is 5'-O-[(S)-hydroxy{[(S)-hydroxy{[(1-hydroxy-2,2,5,5-tetramethyl-2,5-dihydro-1H-pyrrol-3-yl)methyl]disulfanyl}phosphoryl]oxy}phosphoryl]adenosine (three-letter code: JSJ) (formula: $C_{19}H_{30}N_6O_{10}P_2S_2$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 39	C 19	N 6	O 10	P 2	S 2	0	0
3	B	1	Total 39	C 19	N 6	O 10	P 2	S 2	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

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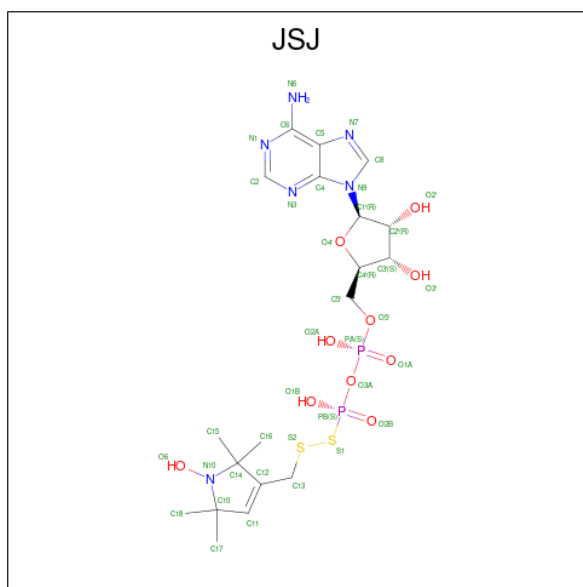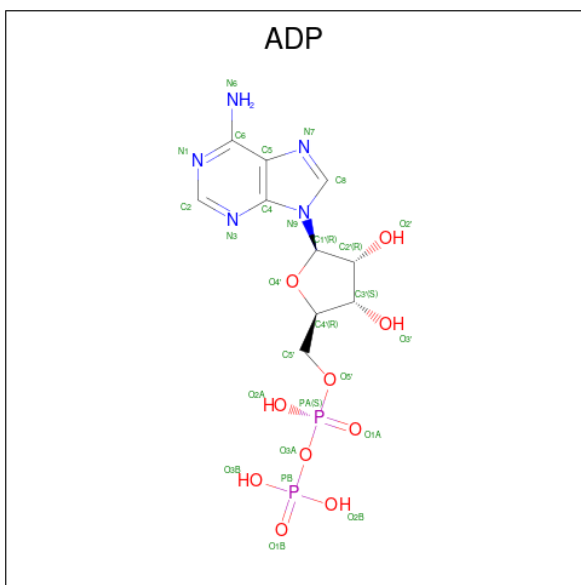
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots ⓘ

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. 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. 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: Chemotaxis protein CheA

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V500 S501 G502 R503 G504 V505 G506 M507 D508 V509 V510 K511 N512 V513 V514 E515 S516 I521 S522 I523 T531 K532 V533 T534 I535 R536 L537 P538 L539

• Molecule 1: Chemotaxis protein CheA

Chain D:

4%

42% 47% 5% 6%

I353 V356 P357 I358 V361 F365 P366 R367 M368 V369 R370 D371 L372 A373 M376 N377 K378 E379 V380 N381 F382 I383 M384 R385 G386 E387 L391 D392 R393 T394 F395 V396 I399 G400 E401 P402 L403 L404 H405 L406 A410 I411 I415 E416 P417 E420 R421 I422 K426 P427

P428 I429 G430 T431 L432 I433 L434 S435 A436 R437 N441 N442 V443 V444 D449 D450 G451 I454 D455 K456 E457 K458 I459 I460 R461 I464 E465 K466 D470 A474 L477 S478 D479 Q480 E481 I482 L483 N484 F485 L486 F487 VAL PRO GLY PHE SER THR LYS GLU LYS VAL SER GLU

V500 V505 G506 M507 D508 K511 N512 V513 V514 E515 S516 L517 N518 G519 S520 I521 S522 I523 E524 S525 E526 G530 T531 K532 V533 T534 I535 R536 L537 P538 L539

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.70Å 75.14Å 86.58Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	10.00 – 2.95 10.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.1 (10.00-2.95) 96.0 (10.00-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	44.77 (at 2.94Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.233 , 0.298 0.229 , 0.292	Depositor DCC
R_{free} test set	19666 reflections (7.92%)	wwPDB-VP
Wilson B-factor (Å^2)	109.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.10 , 79.7	EDS
L-test for twinning [2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.146 for l,k,-h 0.438 for h,-k,-l 0.140 for l,-k,h	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	5687	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, JSJ, SO4

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	0.70	0/1442	0.93	6/1937 (0.3%)
1	B	0.68	1/1450 (0.1%)	0.85	4/1953 (0.2%)
1	C	0.70	1/1406 (0.1%)	0.96	5/1896 (0.3%)
1	D	0.65	0/1303	1.01	9/1761 (0.5%)
All	All	0.68	2/5601 (0.0%)	0.93	24/7547 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	509	VAL	CB-CG1	-9.39	1.33	1.52
1	B	508	ASP	CB-CG	-5.06	1.41	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	508	ASP	CB-CG-OD2	-11.74	107.74	118.30
1	D	421	ARG	NE-CZ-NH1	-11.07	114.76	120.30
1	C	408	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	D	353	ILE	CG1-CB-CG2	-9.38	90.76	111.40
1	D	421	ARG	NE-CZ-NH2	8.59	124.60	120.30
1	A	354	ARG	CD-NE-CZ	8.17	135.04	123.60
1	D	370	ARG	CG-CD-NE	-7.89	95.24	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	391	LEU	CB-CG-CD2	-7.82	97.70	111.00
1	A	354	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	354	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	483	LEU	CB-CG-CD2	-6.71	99.59	111.00
1	B	517	LEU	CB-CG-CD2	-6.69	99.62	111.00
1	A	508	ASP	CB-CA-C	-6.30	97.81	110.40
1	D	370	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	482	ILE	CG1-CB-CG2	-5.76	98.72	111.40
1	B	391	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	D	432	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	C	372	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	A	354	ARG	CB-CA-C	5.50	121.39	110.40
1	D	376	MET	CB-CG-SD	5.46	128.78	112.40
1	C	483	LEU	CA-CB-CG	5.29	127.46	115.30
1	D	486	LEU	CA-CB-CG	5.22	127.32	115.30
1	B	486	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	B	432	LEU	CB-CG-CD1	-5.17	102.20	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	511	LYS	Peptide

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	1425	0	1462	83	0
1	B	1432	0	1452	94	0
1	C	1390	0	1372	111	0
1	D	1288	0	1243	104	0
2	A	10	0	0	2	0
2	C	10	0	0	2	0
3	A	39	0	0	0	0
3	B	39	0	0	2	0
4	C	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	27	0	12	3	0
All	All	5687	0	5553	379	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 34.

All (379) 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:C:478:SER:C	1:C:482:ILE:HD13	1.69	1.13
1:D:454:ILE:HD13	1:D:531:THR:HG21	1.29	1.12
1:B:424:LYS:NZ	1:B:528:ASP:OD2	1.91	1.02
1:A:479:ASP:OD1	1:B:536:ARG:NH1	1.92	1.01
1:C:505:VAL:HB	1:C:509:VAL:HG11	1.40	1.01
1:D:356:VAL:HG12	1:D:357:PRO:HD2	1.44	0.98
1:D:456:LYS:NZ	1:D:525:SER:O	1.95	0.97
1:C:421:ARG:NH2	1:C:450:ASP:O	1.98	0.96
1:D:523:ILE:HD13	1:D:533:VAL:HG13	1.51	0.93
1:D:508:ASP:O	1:D:512:ASN:N	2.02	0.93
1:B:409:ASN:ND2	3:B:601:JSJ:O2A	2.02	0.90
1:C:421:ARG:NH1	1:C:427:PRO:O	2.06	0.89
1:A:464:ILE:HD12	1:A:465:GLU:N	1.90	0.85
1:D:378:LYS:HD2	1:D:417:PRO:HA	1.60	0.84
1:C:395:PHE:O	1:C:399:ILE:HG13	1.78	0.83
1:C:437:ARG:NH1	1:C:446:GLU:OE1	2.11	0.83
1:C:380:VAL:HG11	1:C:411:ILE:HG23	1.61	0.81
1:C:395:PHE:HB3	1:C:399:ILE:HD11	1.62	0.81
1:C:478:SER:O	1:C:482:ILE:HD13	1.81	0.80
1:B:510:VAL:O	1:B:514:VAL:HG23	1.82	0.78
1:A:456:LYS:NZ	2:A:603:SO4:O2	2.19	0.76
1:C:505:VAL:CB	1:C:509:VAL:HG11	2.16	0.76
1:D:392:ASP:OD2	1:D:393:ARG:N	2.19	0.75
1:A:536:ARG:NH2	1:B:457:GLU:OE2	2.20	0.75
1:D:401:GLU:HA	1:D:404:LEU:HB2	1.68	0.75
1:D:421:ARG:HH12	1:D:429:ILE:C	1.90	0.75
1:D:368:MET:SD	1:D:404:LEU:HD21	2.27	0.75
1:C:454:ILE:HD11	4:C:602:ADP:C5	2.22	0.75
1:A:512:ASN:O	1:A:516:SER:N	2.21	0.74
1:D:454:ILE:CD1	1:D:531:THR:HG21	2.15	0.74
1:D:356:VAL:CG1	1:D:357:PRO:HD2	2.18	0.73
1:A:416:GLU:OE2	1:A:426:LYS:NZ	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:VAL:HG21	1:D:432:LEU:HD23	1.71	0.73
1:C:475:ALA:HB2	1:D:442:ASN:HD21	1.53	0.72
1:A:487:PHE:HZ	1:A:521:ILE:HD13	1.54	0.72
1:D:474:ALA:HA	1:D:477:LEU:HD23	1.72	0.71
1:B:504:GLY:H	1:C:401:GLU:HB2	1.55	0.71
1:B:390:GLU:N	1:B:390:GLU:OE2	2.24	0.70
1:B:451:GLY:H	1:B:530:GLY:HA2	1.54	0.70
1:C:372:LEU:HD21	1:C:408:ARG:HG3	1.74	0.69
1:A:487:PHE:CZ	1:A:521:ILE:HD13	2.27	0.69
1:A:409:ASN:O	1:A:413:HIS:N	2.24	0.69
1:B:379:GLU:H	1:B:418:LYS:HZ1	1.41	0.69
1:B:391:LEU:HD21	1:B:443:VAL:HG11	1.74	0.69
1:D:402:PRO:O	1:D:406:LEU:HD12	1.92	0.69
1:D:535:ILE:HG22	1:D:537:LEU:HD11	1.75	0.69
1:C:477:LEU:HB3	1:C:482:ILE:HD12	1.75	0.68
1:C:438:HIS:O	1:C:438:HIS:ND1	2.27	0.68
1:D:380:VAL:HG11	1:D:411:ILE:HD11	1.75	0.68
1:C:449:ASP:OD1	1:C:531:THR:N	2.26	0.68
1:D:460:ILE:O	1:D:464:ILE:N	2.24	0.68
1:C:478:SER:O	1:C:482:ILE:N	2.20	0.67
1:B:404:LEU:HD23	1:B:404:LEU:O	1.93	0.67
1:B:439:GLU:OE1	1:B:536:ARG:NH2	2.28	0.67
1:C:511:LYS:HG2	1:C:511:LYS:O	1.93	0.67
1:B:402:PRO:HB3	1:B:510:VAL:HG13	1.77	0.67
1:B:462:LYS:O	1:B:466:LYS:HB2	1.94	0.67
1:A:365:PHE:HE2	1:A:404:LEU:HG	1.59	0.67
1:D:478:SER:O	1:D:482:ILE:HG13	1.94	0.67
1:C:390:GLU:O	1:C:391:LEU:HD23	1.95	0.66
1:A:514:VAL:HG12	1:A:519:GLY:C	2.15	0.66
1:B:391:LEU:HD11	1:B:445:ILE:HD11	1.77	0.66
1:A:368:MET:SD	1:A:404:LEU:HD11	2.35	0.66
1:A:480:GLN:OE1	1:B:480:GLN:HB3	1.96	0.66
1:C:402:PRO:HG3	1:C:513:VAL:HG11	1.78	0.66
1:D:523:ILE:CD1	1:D:533:VAL:HG13	2.26	0.65
1:A:477:LEU:HD13	1:A:482:ILE:HG12	1.77	0.65
1:A:416:GLU:HG2	1:A:452:ARG:NH1	2.12	0.65
1:B:395:PHE:O	1:B:399:ILE:HG13	1.97	0.64
1:D:395:PHE:HB3	1:D:399:ILE:HD11	1.79	0.64
1:C:506:GLY:C	1:C:508:ASP:N	2.49	0.64
1:D:454:ILE:HD11	4:D:601:ADP:C5	2.33	0.64
1:B:509:VAL:HG21	1:C:509:VAL:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:MET:CE	1:C:502:GLY:HA3	2.29	0.63
1:C:405:HIS:CD2	1:C:409:ASN:OD1	2.52	0.63
1:C:463:ALA:O	1:C:467:GLY:N	2.28	0.63
1:D:416:GLU:N	1:D:416:GLU:OE2	2.31	0.63
1:A:443:VAL:O	1:A:537:LEU:N	2.31	0.63
1:C:506:GLY:O	1:C:509:VAL:HG12	1.99	0.63
1:C:361:VAL:HG13	1:C:362:PHE:HD1	1.64	0.63
1:B:466:LYS:HB3	1:B:468:LEU:HD23	1.81	0.63
1:D:365:PHE:CE1	1:D:404:LEU:HD11	2.33	0.62
1:B:354:ARG:HE	1:B:355:MET:H	1.47	0.62
1:B:448:GLU:HG2	1:B:532:LYS:HG3	1.80	0.62
1:B:506:GLY:O	1:B:509:VAL:HG12	2.00	0.62
1:A:366:PRO:O	1:A:370:ARG:HG3	1.99	0.62
1:D:482:ILE:O	1:D:485:PHE:HB2	2.00	0.62
1:C:487:PHE:HE2	1:C:521:ILE:HG21	1.66	0.61
1:C:483:LEU:HG	1:C:523:ILE:HG13	1.82	0.61
1:B:415:ILE:HD12	1:B:430:GLY:HA3	1.82	0.61
1:C:421:ARG:NH2	1:C:426:LYS:HD3	2.16	0.61
1:C:487:PHE:CD1	1:C:507:MET:HB3	2.36	0.61
1:D:436:ALA:HA	1:D:444:VAL:O	2.00	0.61
1:D:395:PHE:HE2	1:D:517:LEU:HD22	1.66	0.61
1:D:487:PHE:HE2	1:D:523:ILE:HD11	1.66	0.61
1:B:420:GLU:OE2	1:B:452:ARG:NH2	2.32	0.60
1:D:377:ASN:O	1:D:378:LYS:HE2	2.01	0.60
1:A:510:VAL:O	1:A:514:VAL:HG23	2.01	0.60
1:D:455:ASP:HB3	1:D:458:LYS:HB2	1.82	0.60
1:A:365:PHE:CE2	1:A:404:LEU:HG	2.36	0.60
1:C:382:PHE:CE2	1:C:384:MET:HE3	2.37	0.60
1:D:416:GLU:HB2	1:D:421:ARG:CG	2.32	0.60
1:C:489:PRO:HG3	1:C:508:ASP:OD2	2.01	0.60
1:D:454:ILE:HD11	4:D:601:ADP:C6	2.37	0.60
1:B:513:VAL:O	1:B:517:LEU:HD12	2.02	0.59
1:C:433:ILE:O	1:C:447:VAL:HA	2.01	0.59
1:A:407:LEU:O	1:A:411:ILE:HD12	2.02	0.59
1:B:399:ILE:O	1:B:402:PRO:HD2	2.03	0.59
1:B:424:LYS:NZ	1:B:528:ASP:CG	2.56	0.59
1:C:487:PHE:CD2	1:C:511:LYS:HB2	2.38	0.59
1:D:480:GLN:O	1:D:484:ASN:HB2	2.03	0.59
1:C:449:ASP:CG	1:C:531:THR:H	2.06	0.58
1:C:361:VAL:HB	1:C:396:VAL:HG23	1.85	0.58
1:C:391:LEU:HD11	1:C:443:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:ASP:OD2	1:C:471:GLU:N	2.36	0.58
1:D:353:ILE:HG13	1:D:392:ASP:OD1	2.04	0.58
1:D:384:MET:HE3	1:D:387:GLU:OE2	2.04	0.58
1:C:381:ASN:HB3	1:C:431:THR:HA	1.86	0.58
1:B:462:LYS:HD3	1:B:491:PHE:CE2	2.39	0.57
1:B:405:HIS:CD2	1:B:510:VAL:HG21	2.40	0.57
1:B:509:VAL:O	1:B:513:VAL:HG23	2.03	0.57
1:D:521:ILE:HA	1:D:534:THR:O	2.05	0.57
1:C:381:ASN:O	1:C:432:LEU:N	2.27	0.57
1:B:395:PHE:N	1:B:395:PHE:CD1	2.72	0.57
1:C:383:ILE:HB	1:C:433:ILE:HG22	1.86	0.57
1:B:446:GLU:OE1	1:B:532:LYS:HE3	2.05	0.57
1:D:399:ILE:O	1:D:403:LEU:HG	2.05	0.57
1:C:416:GLU:OE1	1:C:452:ARG:N	2.38	0.56
1:B:354:ARG:HA	1:B:354:ARG:NE	2.21	0.56
1:C:483:LEU:HG	1:C:523:ILE:CG1	2.34	0.56
1:C:487:PHE:CE1	1:C:507:MET:HB3	2.39	0.56
1:D:421:ARG:HB3	1:D:426:LYS:HB2	1.87	0.56
1:A:525:SER:OG	1:A:531:THR:HG22	2.05	0.56
1:D:391:LEU:CD2	1:D:443:VAL:HG21	2.36	0.56
1:D:353:ILE:CG1	1:D:392:ASP:OD1	2.53	0.56
1:B:453:GLY:HA2	1:B:531:THR:HG23	1.87	0.56
1:C:535:ILE:HG22	1:C:537:LEU:HD13	1.88	0.56
1:C:478:SER:C	1:C:482:ILE:CD1	2.61	0.56
1:C:522:SER:N	1:C:534:THR:O	2.39	0.55
1:D:507:MET:O	1:D:511:LYS:N	2.29	0.55
1:D:451:GLY:H	1:D:530:GLY:HA2	1.71	0.55
1:A:497:VAL:HG23	1:A:498:SER:H	1.71	0.55
1:C:437:ARG:HB2	1:C:444:VAL:HG22	1.88	0.55
1:B:394:THR:HB	1:B:395:PHE:CD1	2.41	0.55
1:D:380:VAL:CG2	1:D:432:LEU:HD23	2.36	0.55
1:D:416:GLU:HB2	1:D:421:ARG:HG2	1.88	0.54
1:D:410:ALA:O	1:D:415:ILE:N	2.39	0.54
1:B:514:VAL:HG13	1:B:535:ILE:HG23	1.90	0.54
1:D:372:LEU:HD12	1:D:372:LEU:H	1.72	0.54
1:D:395:PHE:CE2	1:D:517:LEU:HD22	2.41	0.54
1:B:484:ASN:O	1:B:487:PHE:HB2	2.08	0.54
1:D:457:GLU:O	1:D:461:ARG:N	2.36	0.54
1:A:446:GLU:HG2	1:A:534:THR:HG23	1.89	0.54
1:C:521:ILE:HA	1:C:534:THR:O	2.08	0.54
1:C:507:MET:HG2	4:C:602:ADP:O2A	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:VAL:HG21	1:B:396:VAL:O	2.09	0.53
1:C:478:SER:O	1:C:482:ILE:CD1	2.56	0.53
1:C:390:GLU:C	1:C:391:LEU:HD23	2.29	0.53
1:D:454:ILE:HD13	1:D:531:THR:CG2	2.20	0.53
1:A:483:LEU:HA	1:A:486:LEU:HD13	1.91	0.53
1:B:536:ARG:O	1:B:537:LEU:HD23	2.09	0.53
1:A:464:ILE:CD1	1:A:465:GLU:N	2.69	0.53
1:A:476:THR:O	1:B:520:SER:OG	2.24	0.53
1:A:514:VAL:HG13	1:A:535:ILE:HG23	1.90	0.53
1:C:459:ILE:CD1	1:C:486:LEU:HD21	2.39	0.53
1:C:483:LEU:HD12	1:C:486:LEU:HD11	1.91	0.53
1:D:366:PRO:O	1:D:369:VAL:HG12	2.07	0.53
1:B:466:LYS:HB3	1:B:468:LEU:CD2	2.39	0.53
1:C:509:VAL:N	1:C:512:ASN:ND2	2.57	0.52
1:C:447:VAL:HG22	1:C:533:VAL:HG22	1.90	0.52
1:C:510:VAL:O	1:C:514:VAL:HG13	2.08	0.52
1:A:516:SER:OG	1:A:517:LEU:HG	2.09	0.52
1:B:403:LEU:O	1:B:407:LEU:HG	2.10	0.52
1:A:416:GLU:HG3	1:A:452:ARG:HG2	1.90	0.52
1:A:480:GLN:HB3	1:B:480:GLN:NE2	2.23	0.52
1:B:399:ILE:C	1:B:402:PRO:HD2	2.31	0.51
1:D:403:LEU:HA	1:D:406:LEU:HD13	1.92	0.51
1:D:391:LEU:HG	1:D:443:VAL:HG11	1.93	0.51
1:D:525:SER:HB2	1:D:531:THR:HG22	1.93	0.51
1:C:511:LYS:N	1:C:512:ASN:ND2	2.59	0.51
1:A:486:LEU:N	1:A:486:LEU:HD12	2.26	0.51
1:C:435:SER:O	1:C:445:ILE:HA	2.10	0.51
1:A:373:ALA:HB3	1:A:374:LYS:HE2	1.93	0.51
1:A:409:ASN:OD1	1:A:409:ASN:N	2.26	0.51
1:A:459:ILE:HG12	1:A:486:LEU:HD11	1.92	0.51
1:B:368:MET:HE1	1:C:502:GLY:HA3	1.93	0.51
1:B:519:GLY:HA2	1:B:536:ARG:O	2.11	0.51
1:C:441:ASN:O	1:C:538:PRO:HA	2.10	0.51
1:D:451:GLY:H	1:D:530:GLY:CA	2.23	0.51
1:C:407:LEU:O	1:C:411:ILE:HG13	2.12	0.50
1:B:482:ILE:O	1:B:485:PHE:HB2	2.11	0.50
1:D:421:ARG:CZ	1:D:427:PRO:O	2.59	0.50
1:C:391:LEU:HD21	1:C:443:VAL:CB	2.41	0.50
1:A:482:ILE:O	1:A:485:PHE:HB2	2.11	0.50
1:B:521:ILE:HA	1:B:534:THR:O	2.12	0.50
1:A:405:HIS:O	1:A:409:ASN:OD1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:PRO:HD3	1:C:384:MET:HE1	1.92	0.50
1:B:372:LEU:HD23	1:B:408:ARG:HG3	1.93	0.50
1:A:402:PRO:HA	1:A:510:VAL:HG22	1.94	0.49
1:C:459:ILE:HD13	1:C:486:LEU:HD21	1.93	0.49
1:A:362:PHE:CD1	1:A:434:LEU:HD21	2.47	0.49
1:B:398:GLU:OE1	1:B:517:LEU:HD21	2.12	0.49
1:B:396:VAL:HG13	1:B:397:GLU:H	1.76	0.49
1:D:487:PHE:CE2	1:D:523:ILE:HD11	2.46	0.49
1:D:454:ILE:N	1:D:454:ILE:HD12	2.28	0.49
1:B:362:PHE:CZ	1:B:434:LEU:HD22	2.48	0.49
1:D:391:LEU:HD23	1:D:443:VAL:HG21	1.93	0.49
1:D:421:ARG:O	1:D:426:LYS:N	2.41	0.49
1:B:354:ARG:HE	1:B:354:ARG:HA	1.77	0.49
1:A:399:ILE:C	1:A:402:PRO:HD2	2.32	0.49
1:B:407:LEU:O	1:B:411:ILE:HG13	2.13	0.49
1:C:523:ILE:HA	1:C:533:VAL:HA	1.93	0.48
1:A:416:GLU:CG	1:A:452:ARG:HG2	2.42	0.48
1:B:464:ILE:HG22	1:B:471:GLU:HA	1.95	0.48
1:D:406:LEU:HD23	1:D:533:VAL:HB	1.94	0.48
1:D:422:ILE:HG13	1:D:422:ILE:O	2.13	0.48
1:B:382:PHE:HD1	1:B:432:LEU:O	1.96	0.48
1:C:487:PHE:CE2	1:C:521:ILE:HG21	2.45	0.48
1:C:506:GLY:C	1:C:508:ASP:H	2.15	0.48
4:C:602:ADP:N3	4:C:602:ADP:H2'	2.27	0.48
1:D:457:GLU:OE1	1:D:461:ARG:NH2	2.47	0.48
1:D:356:VAL:HG12	1:D:357:PRO:CD	2.32	0.48
1:B:460:ILE:HG12	1:B:482:ILE:HD12	1.95	0.48
1:B:502:GLY:HA2	1:C:368:MET:HE1	1.96	0.48
1:C:393:ARG:HA	1:C:396:VAL:HG12	1.96	0.48
1:C:509:VAL:O	1:C:513:VAL:HG23	2.12	0.48
1:B:407:LEU:HD22	1:B:432:LEU:HD21	1.96	0.47
1:C:416:GLU:OE1	1:C:426:LYS:NZ	2.47	0.47
1:D:372:LEU:O	1:D:376:MET:HG2	2.14	0.47
1:D:382:PHE:CD1	1:D:432:LEU:HD11	2.49	0.47
1:A:478:SER:HB2	1:A:480:GLN:HE21	1.80	0.47
1:B:494:LYS:HB3	3:B:601:JSJ:C16	2.43	0.47
1:C:456:LYS:O	1:C:459:ILE:HB	2.14	0.47
1:C:416:GLU:CD	1:C:416:GLU:H	2.18	0.47
1:D:421:ARG:NH1	1:D:427:PRO:O	2.47	0.47
1:C:478:SER:O	1:C:481:GLU:N	2.48	0.47
1:D:384:MET:HA	1:D:434:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:GLU:HB3	1:D:420:GLU:HB3	1.96	0.47
1:D:454:ILE:HD11	4:D:601:ADP:C4	2.50	0.47
1:A:536:ARG:O	1:A:537:LEU:HD23	2.14	0.47
1:A:487:PHE:CD1	1:A:511:LYS:HB2	2.50	0.47
1:D:372:LEU:HD12	1:D:372:LEU:N	2.29	0.47
1:A:353:ILE:O	1:A:354:ARG:NE	2.47	0.46
1:C:443:VAL:HG13	1:C:443:VAL:O	2.15	0.46
1:B:525:SER:CB	1:B:531:THR:HG22	2.45	0.46
1:C:368:MET:SD	1:C:404:LEU:HD11	2.56	0.46
1:B:405:HIS:HD2	1:B:510:VAL:HG21	1.79	0.46
1:C:448:GLU:HB2	1:C:532:LYS:HB2	1.97	0.46
1:B:378:LYS:HE3	1:B:418:LYS:HG2	1.98	0.46
1:C:391:LEU:CD2	1:C:443:VAL:HG11	2.45	0.46
1:C:437:ARG:O	1:C:443:VAL:HA	2.15	0.46
1:D:370:ARG:O	1:D:371:ASP:C	2.54	0.46
1:B:401:GLU:HB3	1:B:402:PRO:HD3	1.97	0.46
1:C:391:LEU:HD21	1:C:443:VAL:HB	1.98	0.46
1:A:483:LEU:HD13	1:A:523:ILE:HG22	1.98	0.46
1:B:514:VAL:HG12	1:B:519:GLY:C	2.36	0.46
1:A:464:ILE:HD12	1:A:464:ILE:C	2.37	0.45
1:C:523:ILE:HG22	1:C:533:VAL:HB	1.98	0.45
1:A:452:ARG:O	1:A:528:ASP:N	2.36	0.45
1:C:535:ILE:HG22	1:C:537:LEU:CD1	2.46	0.45
1:A:385:ARG:HB2	1:A:435:SER:HB3	1.97	0.45
1:A:402:PRO:HG3	1:A:513:VAL:HG21	1.97	0.45
1:A:444:VAL:HA	1:A:535:ILE:O	2.17	0.45
1:D:457:GLU:O	1:D:457:GLU:HG3	2.16	0.45
1:A:480:GLN:HB3	1:B:480:GLN:CD	2.37	0.45
2:C:601:SO4:O2	1:D:526:GLU:HA	2.16	0.45
1:A:364:ARG:HA	1:A:364:ARG:NE	2.31	0.45
1:C:483:LEU:HD23	1:C:523:ILE:O	2.16	0.45
1:A:451:GLY:H	1:A:530:GLY:HA2	1.82	0.45
1:C:511:LYS:C	1:C:514:VAL:HG22	2.37	0.45
1:A:398:GLU:OE1	1:A:513:VAL:HG13	2.17	0.45
1:B:399:ILE:O	1:B:403:LEU:HG	2.17	0.45
1:C:421:ARG:HD3	1:C:427:PRO:O	2.16	0.45
1:C:508:ASP:C	1:C:512:ASN:ND2	2.70	0.45
2:C:601:SO4:O1	1:D:526:GLU:HG3	2.17	0.45
1:D:395:PHE:HE2	1:D:517:LEU:HB3	1.81	0.45
1:B:382:PHE:HA	1:B:432:LEU:O	2.17	0.45
1:A:395:PHE:CD1	1:A:395:PHE:N	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:PHE:HB3	1:A:491:PHE:CE2	2.51	0.44
1:C:361:VAL:HG13	1:C:362:PHE:CD1	2.50	0.44
1:B:474:ALA:O	1:B:477:LEU:HB2	2.17	0.44
1:C:441:ASN:O	1:C:537:LEU:O	2.36	0.44
1:C:468:LEU:HD13	1:C:468:LEU:HA	1.82	0.44
1:C:479:ASP:N	1:C:482:ILE:HD13	2.28	0.44
1:D:437:ARG:O	1:D:444:VAL:HB	2.17	0.44
1:B:468:LEU:HB3	1:B:485:PHE:CE2	2.52	0.44
1:D:365:PHE:N	1:D:366:PRO:HD2	2.33	0.44
1:D:381:ASN:N	1:D:430:GLY:O	2.48	0.44
1:D:449:ASP:OD1	1:D:531:THR:N	2.35	0.44
1:A:475:ALA:O	1:B:520:SER:OG	2.36	0.44
1:D:399:ILE:H	1:D:399:ILE:HG12	1.53	0.44
1:A:384:MET:HA	1:A:434:LEU:O	2.18	0.43
1:A:454:ILE:HD13	1:A:486:LEU:HD21	1.99	0.43
1:D:365:PHE:N	1:D:365:PHE:CD1	2.84	0.43
1:D:373:ALA:HB1	1:D:378:LYS:O	2.18	0.43
1:B:487:PHE:O	1:B:508:ASP:OD1	2.36	0.43
1:D:405:HIS:CE1	1:D:505:VAL:HG13	2.53	0.43
1:C:405:HIS:ND1	1:C:408:ARG:HD3	2.34	0.43
1:C:405:HIS:CE1	1:C:408:ARG:NH1	2.86	0.43
1:C:487:PHE:HE2	1:C:521:ILE:CG2	2.31	0.43
1:A:383:ILE:O	1:A:433:ILE:HA	2.18	0.43
1:A:419:GLU:O	1:A:422:ILE:HG22	2.19	0.43
1:C:449:ASP:OD2	1:C:531:THR:HB	2.18	0.43
1:C:509:VAL:C	1:C:512:ASN:HD22	2.22	0.43
1:A:453:GLY:HA2	1:A:531:THR:CG2	2.48	0.43
1:C:403:LEU:O	1:C:406:LEU:HB2	2.19	0.43
1:A:437:ARG:NH1	2:A:601:SO4:O3	2.51	0.43
1:A:464:ILE:HD12	1:A:465:GLU:CA	2.48	0.43
1:D:383:ILE:HB	1:D:433:ILE:HG12	2.01	0.43
1:D:361:VAL:HG11	1:D:396:VAL:O	2.19	0.43
1:A:374:LYS:HA	1:A:374:LYS:HD3	1.83	0.42
1:B:477:LEU:HD23	1:B:477:LEU:HA	1.68	0.42
1:B:525:SER:HB2	1:B:531:THR:HG22	2.01	0.42
1:C:372:LEU:HD11	1:C:408:ARG:HG3	2.01	0.42
1:C:456:LYS:HA	1:C:459:ILE:HD12	2.00	0.42
1:D:353:ILE:HD13	1:D:353:ILE:HG21	1.63	0.42
1:B:395:PHE:N	1:B:395:PHE:HD1	2.14	0.42
1:D:378:LYS:HE2	1:D:378:LYS:HA	2.01	0.42
1:D:457:GLU:O	1:D:460:ILE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:SER:O	1:C:500:VAL:HG23	2.19	0.42
1:D:365:PHE:O	1:D:369:VAL:N	2.51	0.42
1:D:395:PHE:CE2	1:D:517:LEU:HB3	2.53	0.42
1:D:535:ILE:HG22	1:D:537:LEU:CD1	2.46	0.42
1:A:399:ILE:O	1:A:403:LEU:HG	2.20	0.42
1:B:365:PHE:HE2	1:B:404:LEU:HB2	1.84	0.42
1:B:453:GLY:HA2	1:B:531:THR:CG2	2.49	0.42
1:B:514:VAL:HG12	1:B:519:GLY:O	2.20	0.42
1:A:485:PHE:O	1:A:491:PHE:CD2	2.73	0.42
1:B:372:LEU:N	1:B:372:LEU:HD12	2.34	0.42
1:B:399:ILE:HG22	1:B:403:LEU:HG	2.01	0.42
1:B:443:VAL:N	1:B:537:LEU:O	2.39	0.42
1:D:518:ASN:N	1:D:518:ASN:OD1	2.53	0.42
1:A:459:ILE:HG21	1:A:482:ILE:O	2.19	0.42
1:B:473:LYS:O	1:B:476:THR:HG22	2.19	0.42
1:A:361:VAL:CG1	1:A:396:VAL:HG23	2.49	0.42
1:A:362:PHE:CE1	1:A:434:LEU:HD21	2.54	0.42
1:A:410:ALA:O	1:A:415:ILE:N	2.45	0.42
1:B:458:LYS:HA	1:B:458:LYS:HD3	1.81	0.42
1:A:485:PHE:CD1	1:A:491:PHE:HE2	2.38	0.42
1:A:487:PHE:CE1	1:A:511:LYS:HB2	2.55	0.42
1:C:444:VAL:HG12	1:C:536:ARG:HG3	2.01	0.42
1:A:497:VAL:HG23	1:A:498:SER:N	2.35	0.41
1:B:396:VAL:HG13	1:B:397:GLU:N	2.35	0.41
1:D:391:LEU:CG	1:D:443:VAL:HG11	2.50	0.41
1:B:407:LEU:CD2	1:B:432:LEU:HD21	2.50	0.41
1:B:443:VAL:O	1:B:537:LEU:N	2.46	0.41
1:D:366:PRO:HA	1:D:382:PHE:HD2	1.85	0.41
1:B:489:PRO:HG3	1:B:508:ASP:OD2	2.19	0.41
1:D:481:GLU:O	1:D:485:PHE:N	2.54	0.41
1:D:454:ILE:CD1	1:D:454:ILE:N	2.82	0.41
1:A:468:LEU:HD13	1:A:485:PHE:CE1	2.56	0.41
1:B:483:LEU:HD13	1:B:523:ILE:HG22	2.01	0.41
1:C:438:HIS:O	1:C:438:HIS:CG	2.74	0.41
1:D:391:LEU:HD23	1:D:391:LEU:HA	1.84	0.41
1:D:456:LYS:HD3	1:D:479:ASP:OD1	2.21	0.41
1:C:485:PHE:O	1:C:491:PHE:HE2	2.03	0.41
1:D:385:ARG:HD2	1:D:385:ARG:HA	1.90	0.41
1:D:514:VAL:HG22	1:D:519:GLY:O	2.21	0.41
1:B:376:MET:SD	1:B:412:ASP:OD2	2.79	0.41
1:A:469:ILE:HD12	1:A:469:ILE:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:GLU:H	1:B:419:GLU:HG3	1.58	0.41
1:C:369:VAL:CG2	1:C:407:LEU:HD23	2.51	0.41
1:C:511:LYS:HB3	1:C:512:ASN:HD21	1.85	0.41
1:D:455:ASP:CG	1:D:458:LYS:HG2	2.42	0.41
1:A:392:ASP:OD2	1:A:394:THR:OG1	2.35	0.41
1:A:477:LEU:HD13	1:A:482:ILE:CG1	2.49	0.41
1:A:480:GLN:NE2	1:B:522:SER:OG	2.54	0.41
1:A:483:LEU:O	1:A:486:LEU:HD13	2.20	0.41
1:A:514:VAL:HG11	1:A:521:ILE:N	2.36	0.41
1:C:448:GLU:CG	1:C:449:ASP:N	2.83	0.41
1:D:391:LEU:HD21	1:D:443:VAL:HG21	2.02	0.41
1:C:372:LEU:HD13	1:C:372:LEU:HA	1.87	0.40
1:C:483:LEU:CG	1:C:523:ILE:HG13	2.48	0.40
1:A:488:VAL:HG12	1:A:489:PRO:O	2.21	0.40
1:B:462:LYS:HD3	1:B:491:PHE:HE2	1.83	0.40
1:A:433:ILE:O	1:A:447:VAL:HA	2.21	0.40
1:D:411:ILE:HD12	1:D:411:ILE:HG23	1.77	0.40
1:B:391:LEU:HD23	1:B:391:LEU:HA	1.67	0.40
1:C:401:GLU:N	1:C:402:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	179/187 (96%)	177 (99%)	2 (1%)	0	100	100
1	B	185/187 (99%)	179 (97%)	5 (3%)	1 (0%)	25	50
1	C	178/187 (95%)	169 (95%)	8 (4%)	1 (1%)	22	46
1	D	171/187 (91%)	167 (98%)	2 (1%)	2 (1%)	11	29
All	All	713/748 (95%)	692 (97%)	17 (2%)	4 (1%)	22	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	511	LYS
1	D	400	GLY
1	B	440	GLY
1	D	396	VAL

5.3.2　Protein sidechains ⓘ

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	159/165 (96%)	150 (94%)	9 (6%)	17	39
1	B	157/165 (95%)	152 (97%)	5 (3%)	34	59
1	C	149/165 (90%)	134 (90%)	15 (10%)	6	18
1	D	131/165 (79%)	126 (96%)	5 (4%)	28	53
All	All	596/660 (90%)	562 (94%)	34 (6%)	17	39

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ARG
1	A	360	PHE
1	A	393	ARG
1	A	404	LEU
1	A	409	ASN
1	A	441	ASN
1	A	477	LEU
1	A	498	SER
1	A	539	LEU
1	B	378	LYS
1	B	392	ASP
1	B	508	ASP
1	B	517	LEU
1	B	539	LEU
1	C	354	ARG
1	C	371	ASP

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Mol	Chain	Res	Type
1	C	372	LEU
1	C	384	MET
1	C	388	ASP
1	C	418	LYS
1	C	435	SER
1	C	438	HIS
1	C	439	GLU
1	C	466	LYS
1	C	491	PHE
1	C	503	ARG
1	C	516	SER
1	C	521	ILE
1	C	532	LYS
1	D	393	ARG
1	D	399	ILE
1	D	465	GLU
1	D	516	SER
1	D	533	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	480	GLN
1	B	405	HIS
1	C	512	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	SO4	C	603	-	4,4,4	0.21	0	6,6,6	0.24	0
2	SO4	A	601	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	C	601	-	4,4,4	0.24	0	6,6,6	0.28	0
4	ADP	C	602	-	24,29,29	0.91	0	29,45,45	1.64	6 (20%)
4	ADP	D	601	-	24,29,29	1.04	3 (12%)	29,45,45	1.88	7 (24%)
3	JSJ	A	602	-	33,42,42	2.55	3 (9%)	35,67,67	1.72	7 (20%)
3	JSJ	B	601	-	33,42,42	2.56	5 (15%)	35,67,67	2.18	9 (25%)
2	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JSJ	A	602	-	-	3/13/62/62	0/4/4/4
3	JSJ	B	601	-	-	7/13/62/62	0/4/4/4
4	ADP	C	602	-	-	5/12/32/32	0/3/3/3
4	ADP	D	601	-	-	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	B	601	JSJ	PB-S1	-11.43	1.88	2.09
3	A	602	JSJ	PB-S1	-11.38	1.88	2.09
3	A	602	JSJ	C13-S2	-7.48	1.71	1.82
3	B	601	JSJ	C13-S2	-7.36	1.71	1.82
4	D	601	ADP	C2-N3	2.36	1.35	1.32
3	A	602	JSJ	PB-O1B	-2.28	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	JSJ	C11-C12	2.26	1.35	1.32
4	D	601	ADP	O4'-C1'	2.16	1.43	1.40
3	B	601	JSJ	PB-O2B	2.16	1.51	1.46
4	D	601	ADP	C6-C5	2.08	1.51	1.43
3	B	601	JSJ	PB-O1B	-2.08	1.51	1.56

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	JSJ	C17-C10-N10	6.74	117.77	110.05
3	A	602	JSJ	C11-C10-N10	4.93	102.82	99.43
4	D	601	ADP	N3-C2-N1	-4.86	122.07	128.67
3	B	601	JSJ	C18-C10-C11	-4.85	108.17	112.77
4	C	602	ADP	N3-C2-N1	-4.35	122.76	128.67
3	B	601	JSJ	C18-C10-N10	-4.28	105.15	110.05
4	D	601	ADP	C4-C5-N7	-4.14	104.96	109.34
3	A	602	JSJ	N3-C2-N1	-3.96	123.30	128.67
3	B	601	JSJ	N3-C2-N1	-3.81	123.50	128.67
4	D	601	ADP	C5'-C4'-C3'	-3.65	102.06	115.21
3	B	601	JSJ	C11-C10-N10	3.50	101.84	99.43
4	C	602	ADP	C4-C5-N7	-3.28	105.87	109.34
3	A	602	JSJ	C17-C10-C11	-3.15	109.78	112.77
3	A	602	JSJ	C4-C5-N7	-3.09	106.08	109.34
4	C	602	ADP	C5'-C4'-C3'	-3.04	104.27	115.21
4	D	601	ADP	O4'-C1'-N9	3.04	112.77	108.75
3	B	601	JSJ	C17-C10-C11	2.99	115.60	112.77
3	B	601	JSJ	C18-C10-C17	-2.67	107.54	110.94
3	A	602	JSJ	C18-C10-C11	-2.59	110.31	112.77
3	A	602	JSJ	C10-C11-C12	-2.55	111.17	113.48
4	C	602	ADP	O4'-C4'-C3'	2.49	110.10	105.15
4	D	601	ADP	O4'-C4'-C3'	2.46	110.04	105.15
3	B	601	JSJ	C4-C5-N7	-2.36	106.85	109.34
3	A	602	JSJ	O1B-PB-O3A	-2.34	100.94	107.27
4	C	602	ADP	O2A-PA-O1A	2.24	122.87	112.44
4	D	601	ADP	C5-C6-N6	2.17	123.62	120.31
3	B	601	JSJ	O2A-PA-O1A	2.16	122.48	112.44
4	C	602	ADP	O4'-C1'-N9	2.12	111.55	108.75
4	D	601	ADP	O2B-PB-O3A	-2.02	97.86	104.64

There are no chirality outliers.
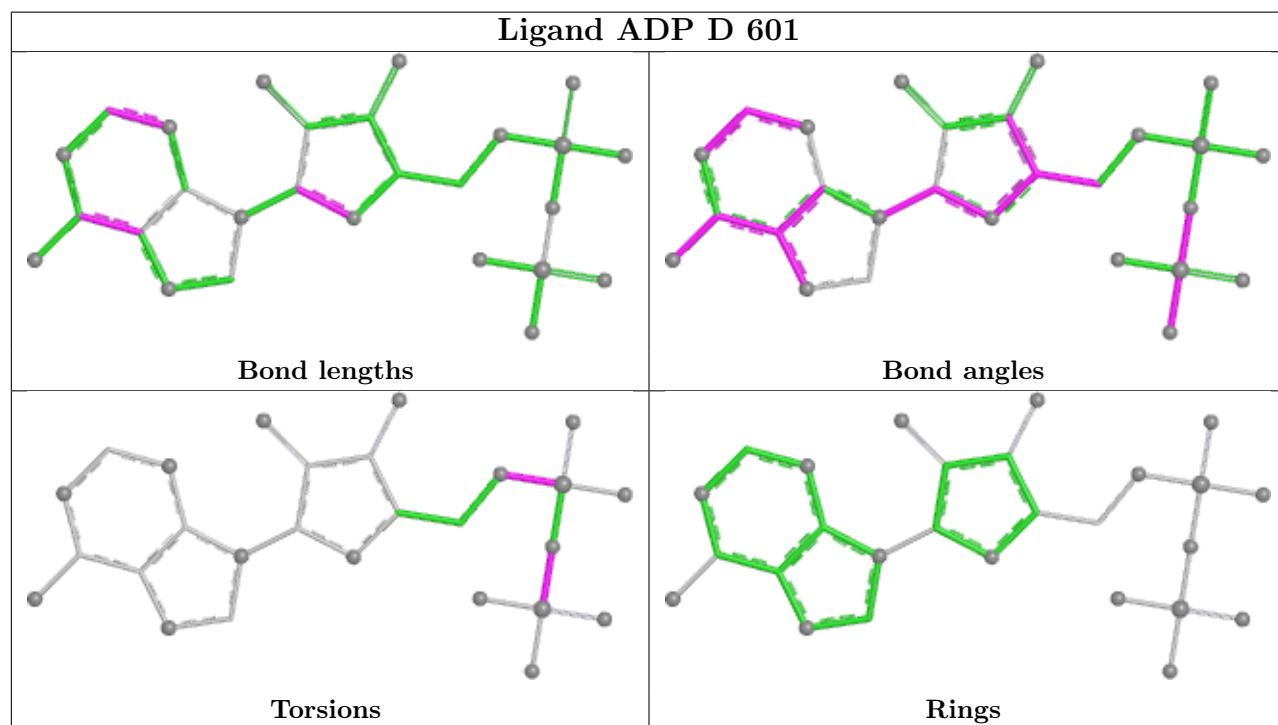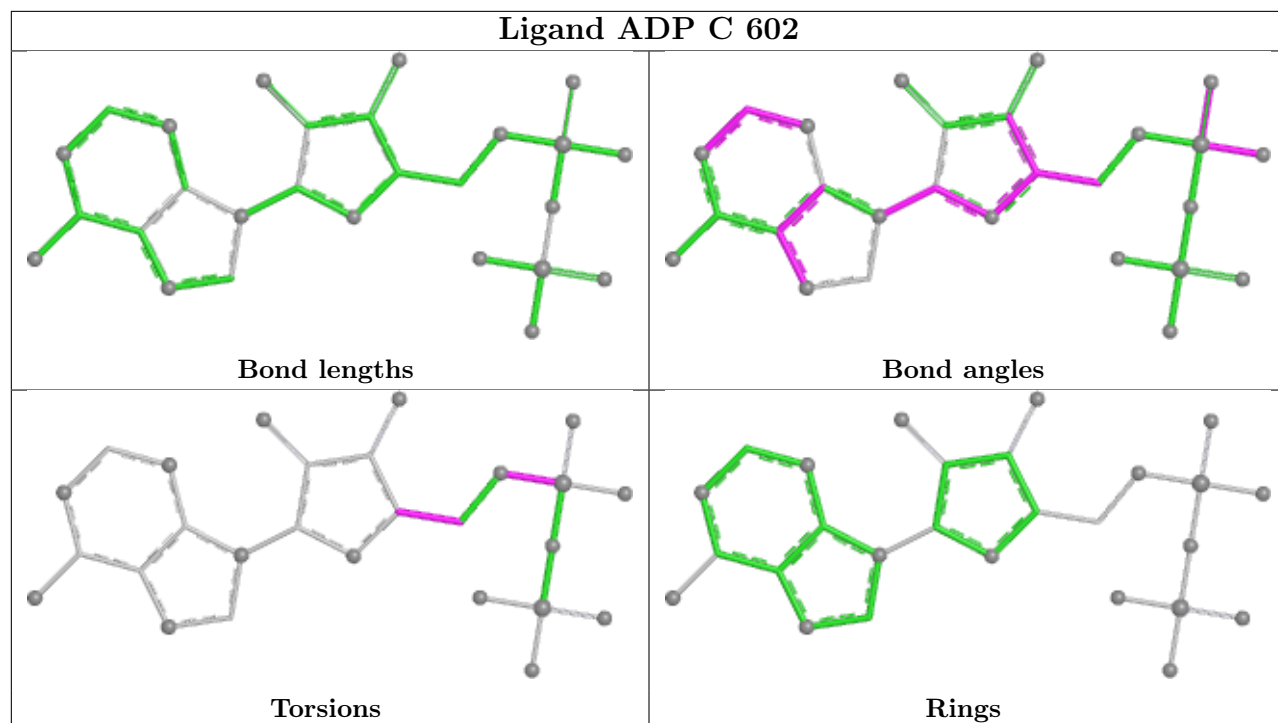
All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	JSJ	C12-C13-S2-S1
3	B	601	JSJ	C11-C12-C13-S2
3	B	601	JSJ	C12-C13-S2-S1
3	B	601	JSJ	C5'-O5'-PA-O3A
4	C	602	ADP	C5'-O5'-PA-O2A
4	C	602	ADP	O4'-C4'-C5'-O5'
4	D	601	ADP	C5'-O5'-PA-O2A
4	D	601	ADP	C5'-O5'-PA-O3A
4	C	602	ADP	C3'-C4'-C5'-O5'
3	A	602	JSJ	C11-C12-C13-S2
3	B	601	JSJ	PB-O3A-PA-O5'
3	B	601	JSJ	PA-O3A-PB-O2B
3	A	602	JSJ	C3'-C4'-C5'-O5'
3	B	601	JSJ	C5'-O5'-PA-O1A
4	C	602	ADP	C5'-O5'-PA-O1A
4	C	602	ADP	C5'-O5'-PA-O3A
4	D	601	ADP	PA-O3A-PB-O1B
3	B	601	JSJ	C4'-C5'-O5'-PA

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SO4	1	0
2	C	601	SO4	2	0
4	C	602	ADP	3	0
4	D	601	ADP	3	0
3	B	601	JSJ	2	0
2	A	603	SO4	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 C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand JSJ A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand JSJ B 601

Bond lengths

Bond angles

Torsions

Rings
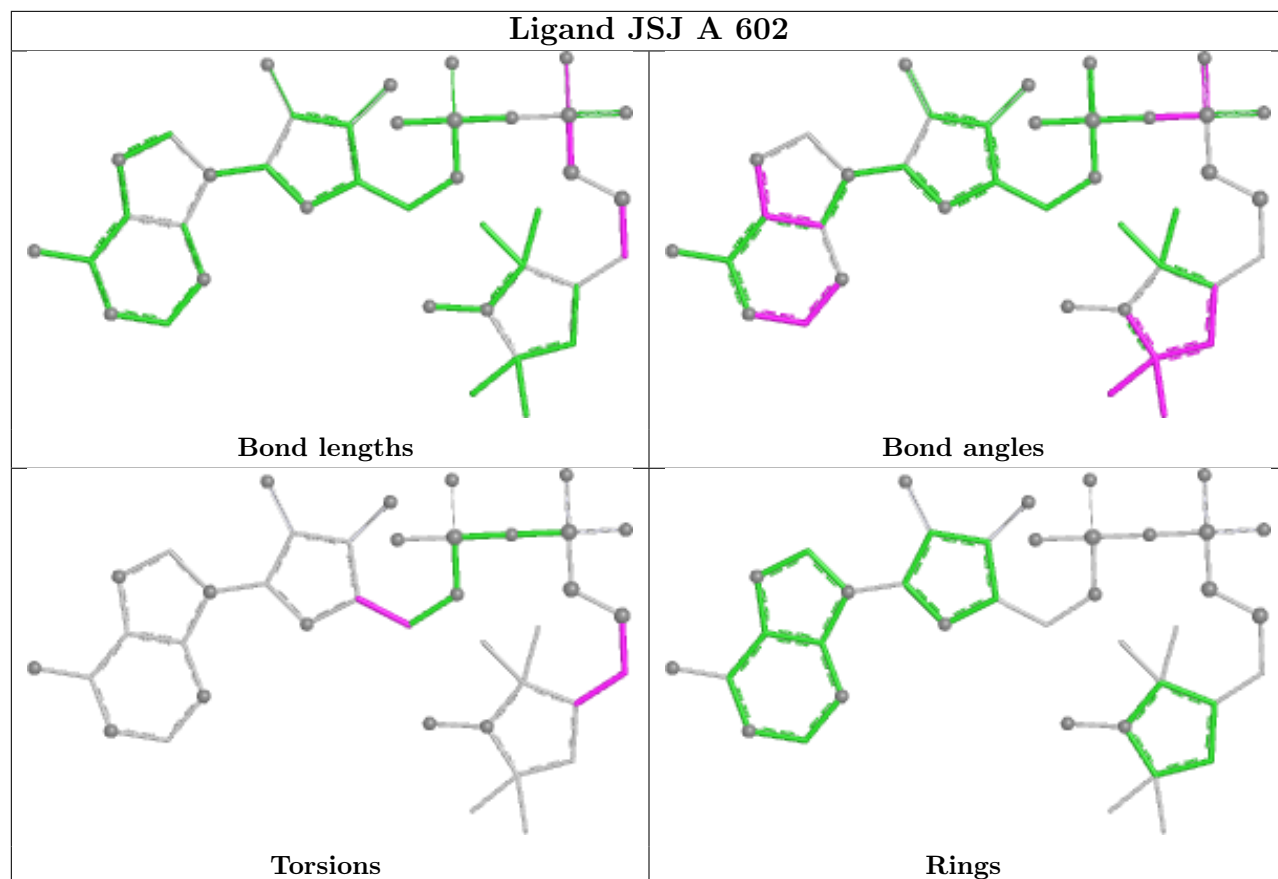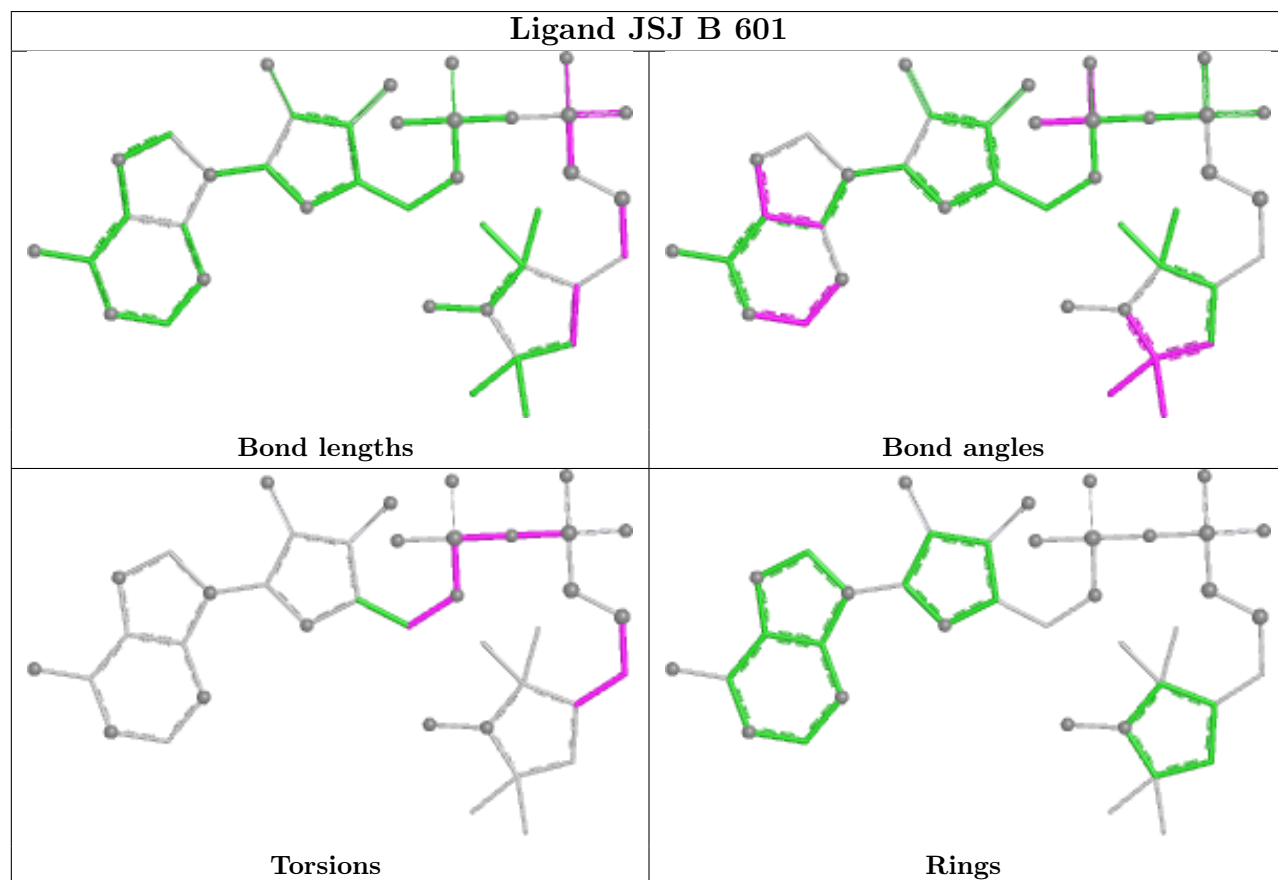
5.7 Other polymers ⓘ

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 ⓘ

Warning: The R factor obtained from EDS is 0.4262, which does not match the depositor's R factor of 0.2325. Please interpret the results in this section carefully.

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(Å²)	Q<0.9
1	A	183/187 (97%)	0.39	11 (6%)	29	26	62, 95, 132, 159	0
1	B	187/187 (100%)	0.54	12 (6%)	27	24	64, 96, 145, 185	0
1	C	184/187 (98%)	0.50	13 (7%)	23	23	67, 109, 145, 167	0
1	D	175/187 (93%)	0.46	8 (4%)	38	35	71, 113, 163, 186	0
All	All	729/748 (97%)	0.47	44 (6%)	29	26	62, 103, 150, 186	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	GLY	8.4
1	C	378	LYS	7.1
1	C	441	ASN	6.5
1	A	453	GLY	6.4
1	A	512	ASN	5.1
1	D	400	GLY	4.7
1	B	508	ASP	4.5
1	C	451	GLY	4.2
1	D	422	ILE	4.1
1	B	401	GLU	3.6
1	A	484	ASN	3.6
1	B	396	VAL	3.2
1	A	464	ILE	3.1
1	D	358	ILE	3.1
1	D	530	GLY	3.0
1	A	511	LYS	3.0
1	B	394	THR	2.9
1	A	409	ASN	2.7
1	D	466	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	441	ASN	2.6
1	A	470	ASP	2.6
1	C	394	THR	2.6
1	C	514	VAL	2.5
1	C	478	SER	2.5
1	C	476	THR	2.5
1	A	463	ALA	2.4
1	C	398	GLU	2.4
1	A	515	GLU	2.3
1	C	401	GLU	2.3
1	A	526	GLU	2.2
1	A	520	SER	2.2
1	B	422	ILE	2.2
1	B	488	VAL	2.2
1	B	490	GLY	2.2
1	C	371	ASP	2.2
1	C	486	LEU	2.2
1	D	428	PRO	2.2
1	B	492	SER	2.2
1	B	525	SER	2.2
1	B	442	ASN	2.0
1	B	425	GLY	2.0
1	C	391	LEU	2.0
1	D	470	ASP	2.0
1	C	457	GLU	2.0

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, 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
2	SO4	A	603	5/5	0.90	0.15	94,98,110,113	0
2	SO4	C	601	5/5	0.90	0.12	95,100,101,102	0
4	ADP	D	601	27/27	0.90	0.12	99,118,126,129	0
4	ADP	C	602	27/27	0.91	0.10	112,134,145,148	0
3	JSJ	A	602	39/39	0.93	0.12	84,113,180,183	0
2	SO4	A	601	5/5	0.96	0.07	92,103,106,109	0
3	JSJ	B	601	39/39	0.96	0.10	79,99,172,174	0
2	SO4	C	603	5/5	0.99	0.06	62,68,76,82	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.
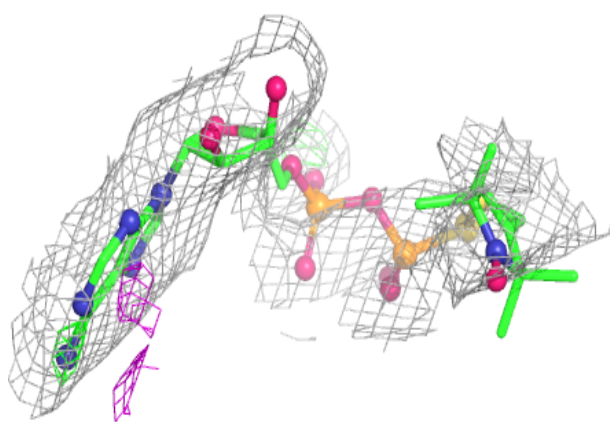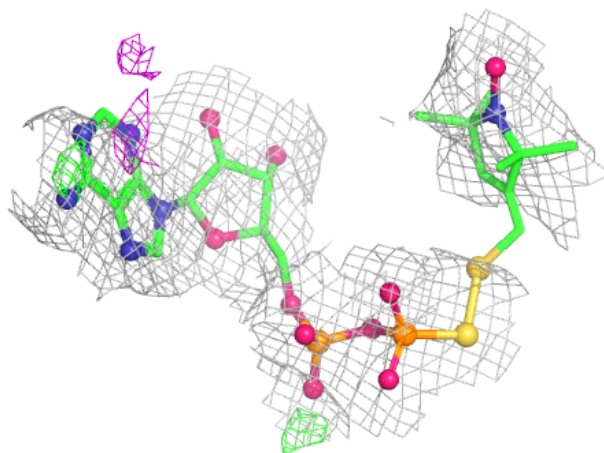
Electron density around ADP D 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
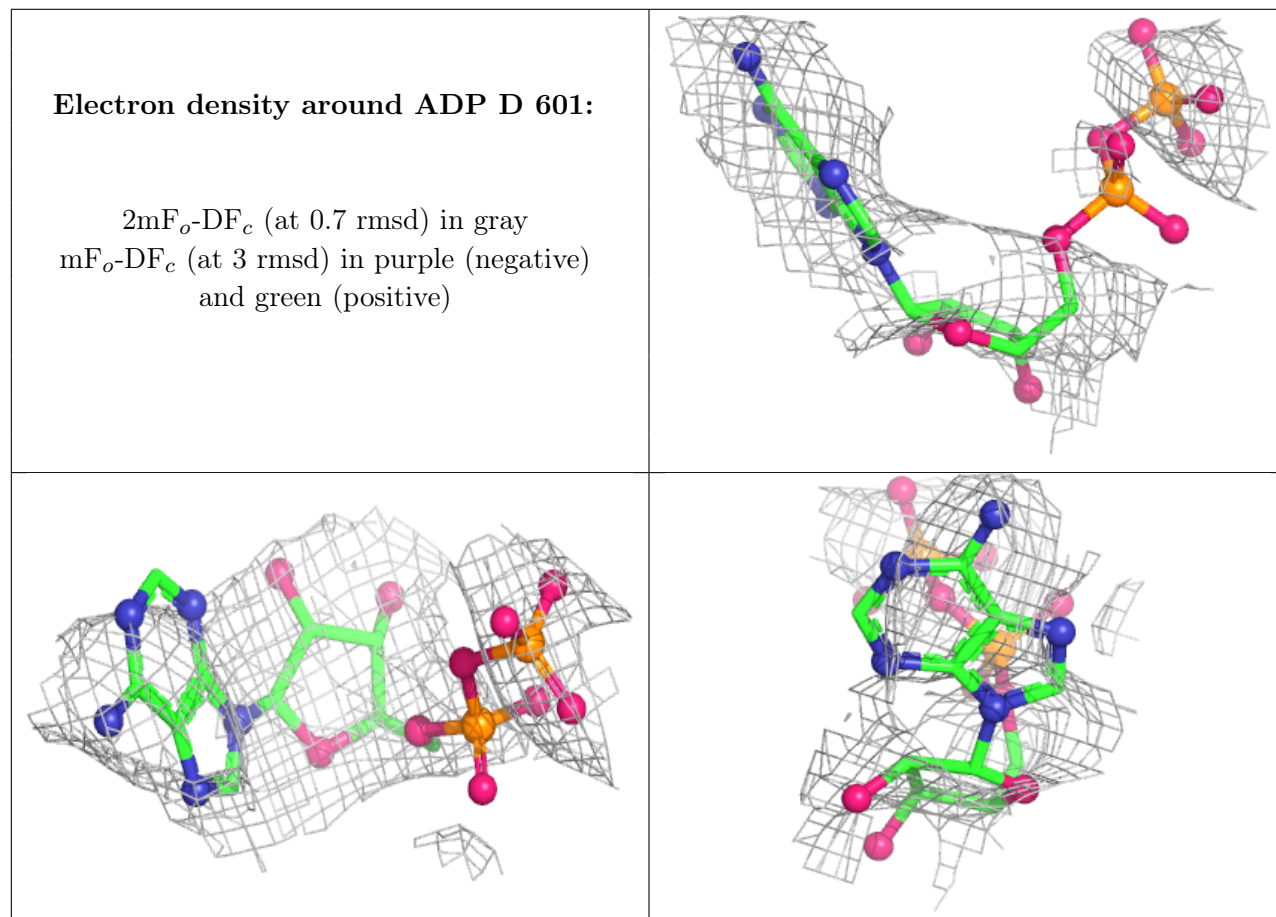
Electron density around ADP C 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
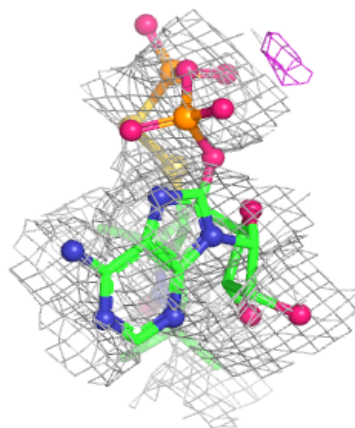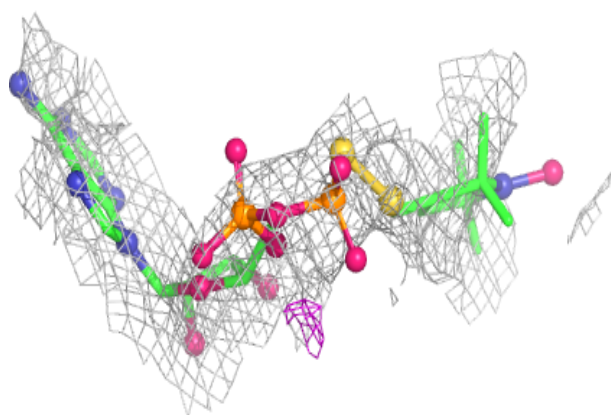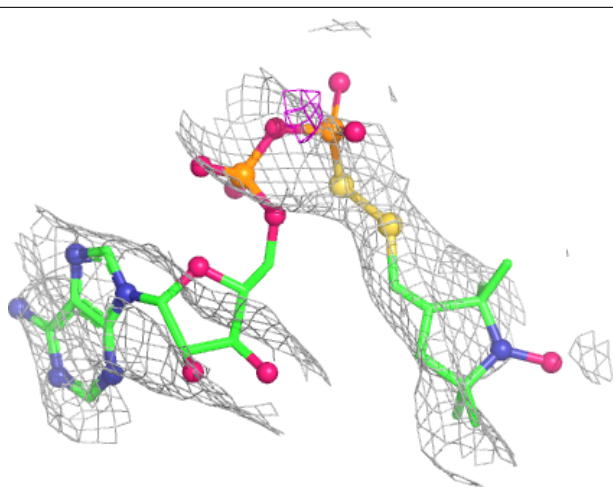and green (positive)
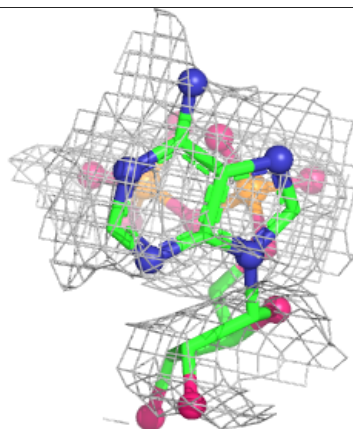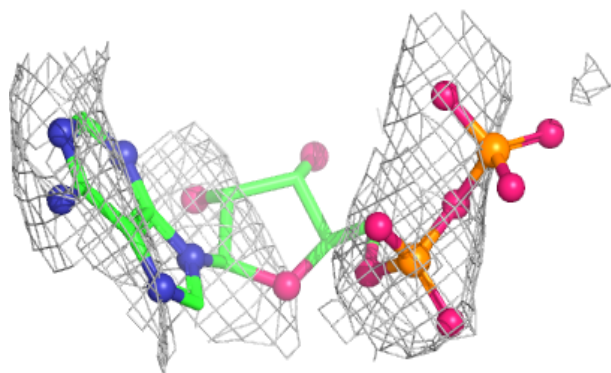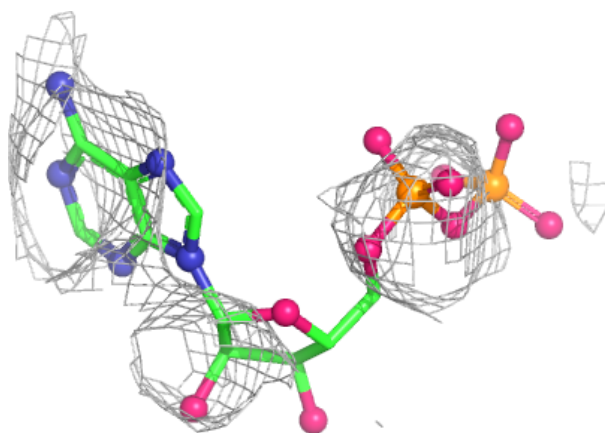
Electron density around JSJ A 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
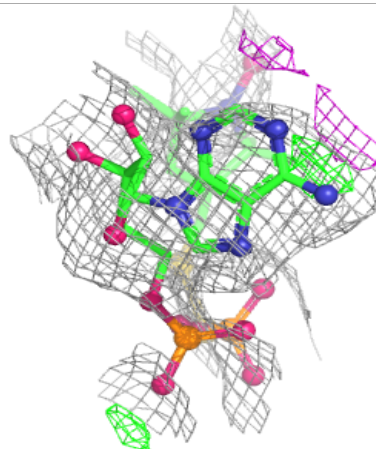
Electron density around JSJ B 601:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.