



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:05 AM UTC

PDB ID : 6MI6 / pdb_00006mi6
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)

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

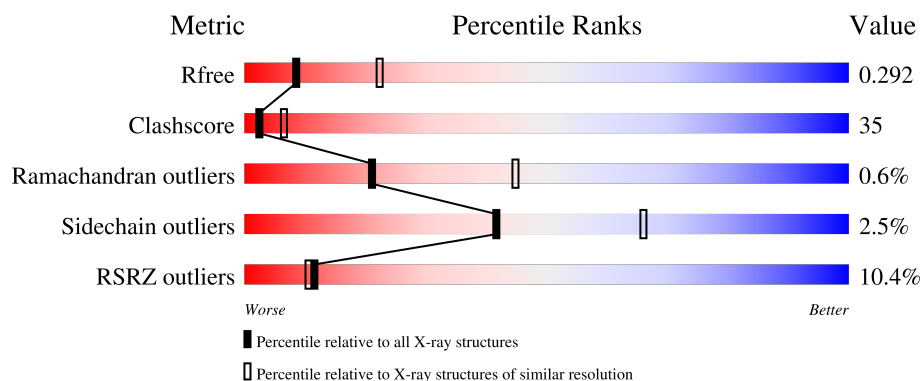
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (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 $\leq 5\%$. 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	187	9% 50% 45% ...
1	B	187	11% 51% 49% .
1	C	187	11% 49% 45% ...
1	D	187	10% 42% 48% . 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 criteria:

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

2 Entry composition [i](#)

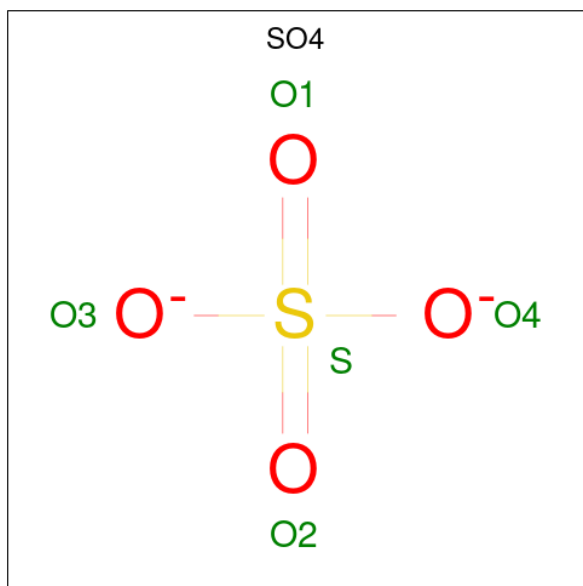
There are 4 unique types of molecules in this entry. The entry contains 5687 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: SO4) (formula: O₄S).



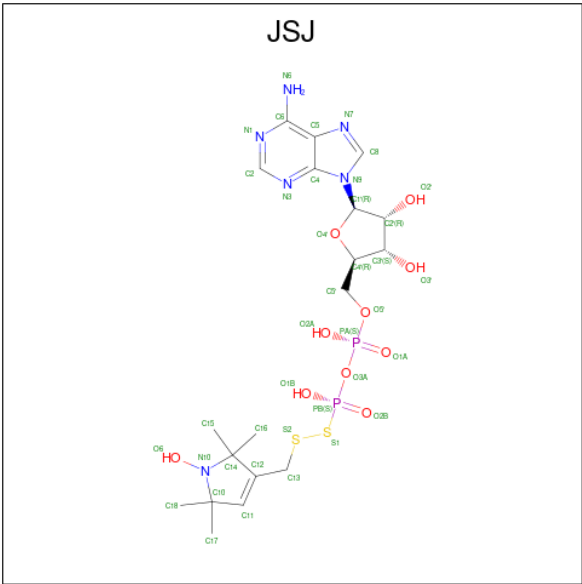
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

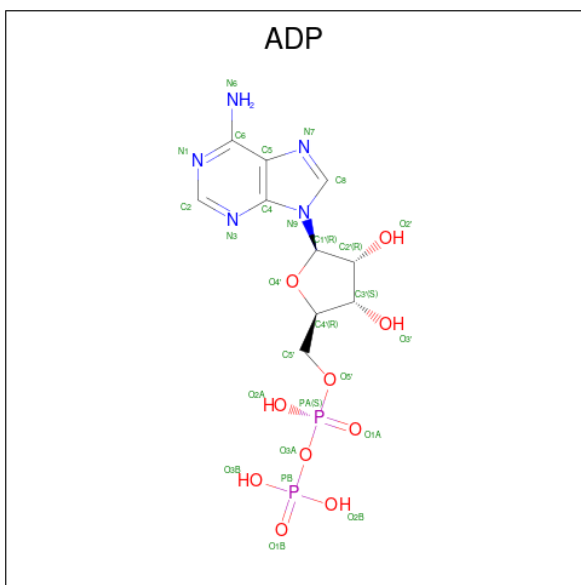
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- 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 (CCD ID: JSJ) (formula: C₁₉H₃₀N₆O₁₀P₂S₂).



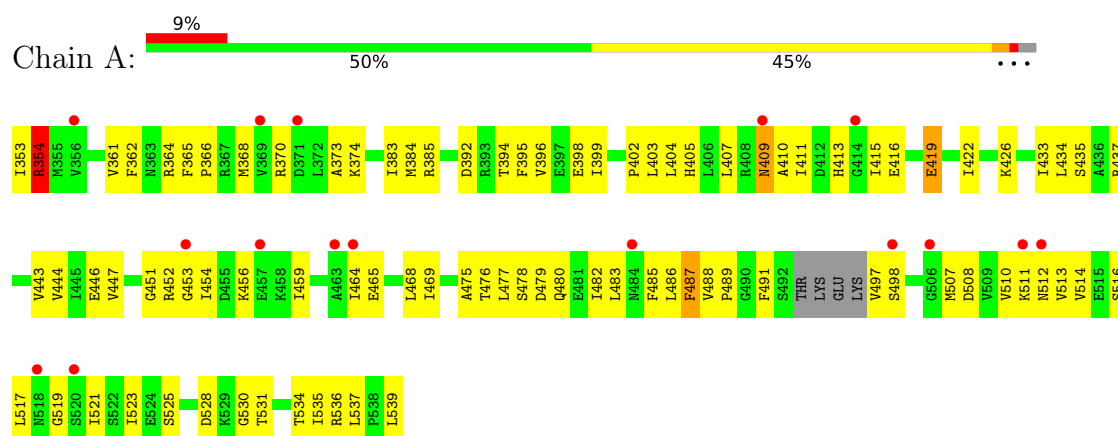


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

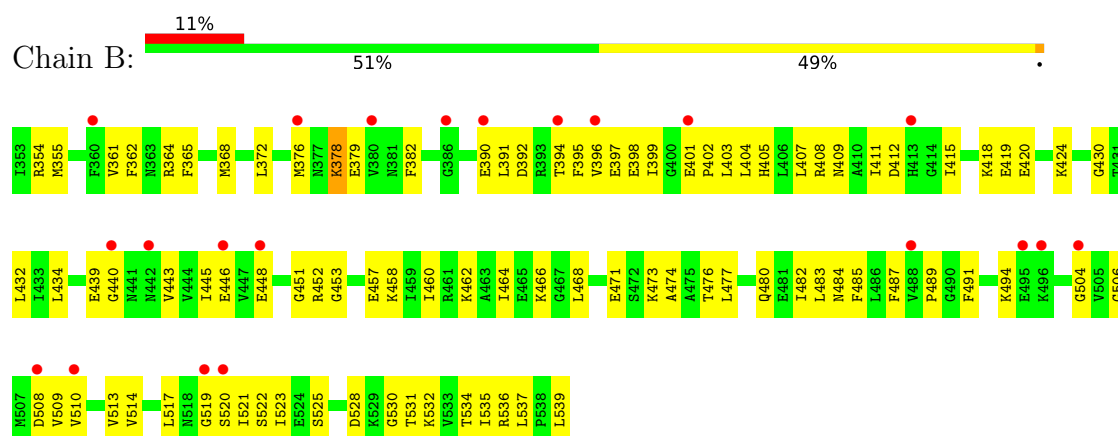
3 Residue-property plots [i](#)

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.

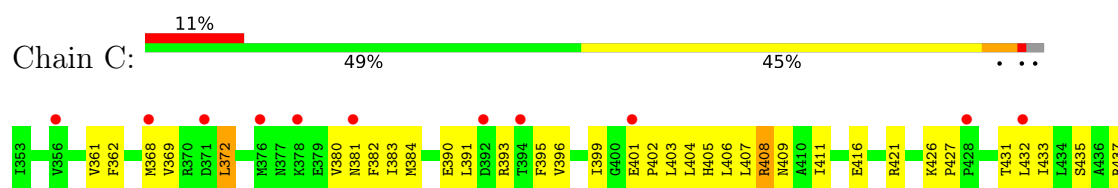
• Molecule 1: Chemotaxis protein CheA

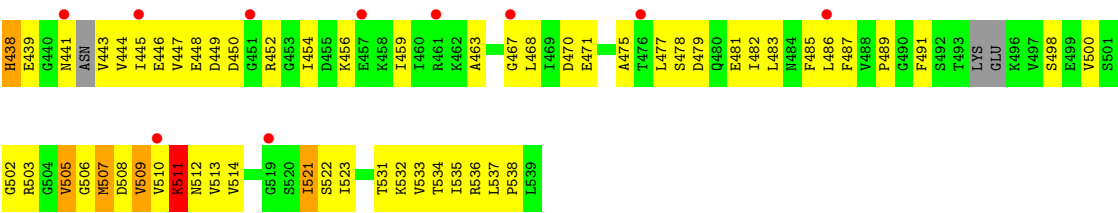


• Molecule 1: Chemotaxis protein CheA

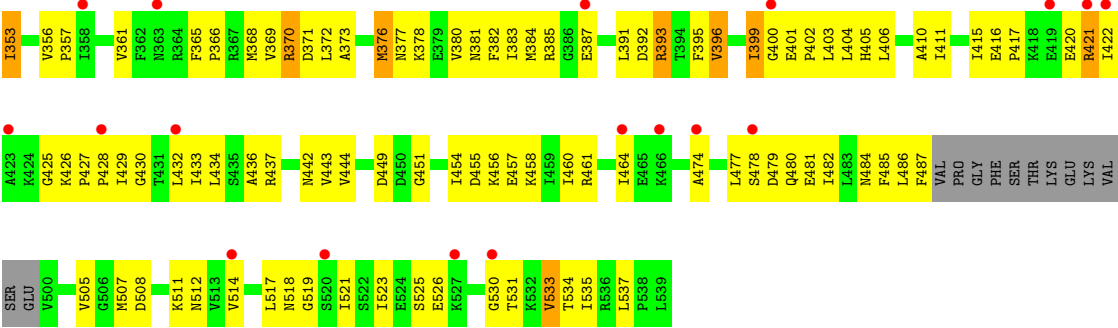


• Molecule 1: Chemotaxis protein CheA





● Molecule 1: Chemotaxis protein CheA



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	2020 reflections (7.80%)	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)	0.08 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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	0.79	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: JSJ, ADP, 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	0.95	9/1937 (0.5%)
1	B	0.69	0/1450	0.92	0/1953
1	C	0.67	1/1406 (0.1%)	1.05	6/1896 (0.3%)
1	D	0.69	1/1303 (0.1%)	1.02	5/1761 (0.3%)
All	All	0.69	2/5601 (0.0%)	0.98	20/7547 (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	-5.89	1.33	1.52
1	D	376	MET	SD-CE	-5.63	1.65	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	507	MET	N-CA-C	-9.14	101.90	112.87
1	D	370	ARG	CG-CD-NE	-7.62	95.24	112.00
1	A	354	ARG	CD-NE-CZ	7.60	135.04	124.40
1	D	421	ARG	NE-CZ-NH1	-6.74	114.76	121.50
1	D	353	ILE	CG1-CB-CG2	-6.65	90.76	110.70
1	C	408	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	A	507	MET	CA-C-N	-6.34	109.91	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	MET	C-N-CA	-6.34	109.91	120.68
1	A	508	ASP	CB-CA-C	-6.16	97.81	110.38
1	A	354	ARG	CB-CA-C	6.08	121.39	109.35
1	D	421	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	A	487	PHE	CA-C-N	-5.84	111.33	122.13
1	A	487	PHE	C-N-CA	-5.84	111.33	122.13
1	C	507	MET	CA-C-N	5.73	132.48	121.54
1	C	507	MET	C-N-CA	5.73	132.48	121.54
1	A	508	ASP	N-CA-CB	5.64	118.99	110.30
1	D	376	MET	CB-CG-SD	5.36	128.78	112.70
1	C	505	VAL	N-CA-C	-5.29	99.99	107.98
1	C	505	VAL	CB-CA-C	5.23	116.87	111.23
1	A	419	GLU	CA-CB-CG	5.10	124.30	114.10

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	97	0
1	C	1390	0	1372	118	0
1	D	1288	0	1243	108	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
4	D	27	0	12	4	0
All	All	5687	0	5553	393	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 35.

All (393) 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	1.17
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:368:MET:HE1	1:C:502:GLY:HA3	1.53	0.91
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:D:421:ARG:HH12	1:D:429:ILE:C	1.90	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: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
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:C:382:PHE:CE2	1:C:384:MET:HE3	2.25	0.71
1:D:474:ALA:HA	1:D:477:LEU:HD23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:VAL:HG12	1:A:519:GLY:C	2.15	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: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:506:GLY:C	1:C:508:ASP:N	2.49	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:B:379:GLU:H	1:B:418:LYS:HZ1	1.42	0.67
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: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:424:LYS:HZ1	1:B:528:ASP:CG	1.99	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: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
1:C:405:HIS:CD2	1:C:409:ASN:OD1	2.52	0.63
1:C:449:ASP:CG	1:C:531:THR:H	2.06	0.63
1:C:463:ALA:O	1:C:467:GLY:N	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:368:MET:CE	1:C:502:GLY:HA3	2.29	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:B:424:LYS:NZ	1:B:528:ASP:CG	2.56	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: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:C:478:SER:C	1:C:482:ILE:CD1	2.61	0.59
1:B:513:VAL:O	1:B:517:LEU:HD12	2.02	0.59
1:D:486:LEU:HD11	1:D:507:MET:HE3	1.84	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: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:390:GLU:C	1:C:391:LEU:HD23	2.29	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
1:C:470:ASP:OD2	1:C:471:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ILE:HG13	1:D:392:ASP:OD1	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:B:399:ILE:C	1:B:402:PRO:HD2	2.31	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: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:C:506:GLY:C	1:C:508:ASP:H	2.15	0.54
1:A:446:GLU:HG2	1:A:534:THR:HG23	1.89	0.54
1:C:362:PHE:O	1:C:384:MET:HE1	2.08	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:D:507:MET:HE1	4:D:601:ADP:H5'1	1.90	0.53
1:A:399:ILE:C	1:A:402:PRO:HD2	2.32	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:D:384:MET:HE3	1:D:387:GLU:OE2	2.08	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:C:416:GLU:CD	1:C:416:GLU:H	2.18	0.52
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:382:PHE:HE2	1:C:384:MET:HE3	1.76	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: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:370:ARG:O	1:D:371:ASP:C	2.54	0.51
1:D:451:GLY:H	1:D:530:GLY:CA	2.23	0.51
1:B:514:VAL:HG12	1:B:519:GLY:C	2.36	0.50
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:A:464:ILE:HD12	1:A:464:ILE:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:480:GLN:HB3	1:B:480:GLN:CD	2.37	0.50
1:B:372:LEU:HD23	1:B:408:ARG:HG3	1.93	0.50
1:C:511:LYS:C	1:C:514:VAL:HG22	2.37	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:C:508:ASP:C	1:C:512:ASN:ND2	2.70	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: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
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:C:393:ARG:HA	1:C:396:VAL:HG12	1.96	0.48
1:C:509:VAL:C	1:C:512:ASN:HD22	2.22	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: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:368:MET:HE1	1:C:502:GLY:CA	2.35	0.47
1:B:494:LYS:HB3	3:B:601:JSJ:C16	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:LYS:O	1:C:459:ILE:HB	2.14	0.47
1:D:421:ARG:NH1	1:D:427:PRO:O	2.47	0.47
1:D:421:ARG:NH1	1:D:429:ILE:C	2.68	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
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:B:364:ARG:O	1:B:368:MET:HE3	2.15	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: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:C:523:ILE:HG22	1:C:533:VAL:HB	1.98	0.45
1:D:455:ASP:CG	1:D:458:LYS:HG2	2.42	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
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:392:ASP:OD2	1:A:394:THR:OG1	2.35	0.45
1:A:451:GLY:H	1:A:530:GLY:HA2	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:439:GLU:CD	1:B:536:ARG:NH2	2.75	0.44
1:B:468:LEU:HB3	1:B:485:PHE:CE2	2.52	0.44
1:C:431:THR:H	1:C:450:ASP:CG	2.23	0.44
1:C:441:ASN:C	1:C:538:PRO:HA	2.43	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:C:510:VAL:C	1:C:512:ASN:H	2.25	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: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:C:509:VAL:C	1:C:512:ASN:HB2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:421:ARG:NH1	1:D:428:PRO:C	2.76	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: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:C:416:GLU:OE1	1:C:426:LYS:NZ	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:399:ILE:C	1:C:402:PRO:HD2	2.46	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
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: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:D:422:ILE:C	1:D:425:GLY:H	2.29	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
1:C:510:VAL:C	1:C:512:ASN:N	2.80	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%)	24	49
1	C	178/187 (95%)	169 (95%)	8 (4%)	1 (1%)	21	45
1	D	171/187 (91%)	167 (98%)	2 (1%)	2 (1%)	10	28
All	All	713/748 (95%)	692 (97%)	17 (2%)	4 (1%)	21	45

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%)	156 (98%)	3 (2%)	50	71
1	B	157/165 (95%)	154 (98%)	3 (2%)	50	71
1	C	149/165 (90%)	144 (97%)	5 (3%)	32	58
1	D	131/165 (79%)	127 (97%)	4 (3%)	35	59
All	All	596/660 (90%)	581 (98%)	15 (2%)	42	66

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ARG
1	A	409	ASN
1	A	539	LEU
1	B	378	LYS
1	B	392	ASP
1	B	539	LEU
1	C	372	LEU

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Mol	Chain	Res	Type
1	C	438	HIS
1	C	439	GLU
1	C	503	ARG
1	C	521	ILE
1	D	393	ARG
1	D	399	ILE
1	D	518	ASN
1	D	533	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	405	HIS
1	A	480	GLN
1	B	405	HIS
1	B	438	HIS
1	B	442	ASN
1	B	480	GLN
1	B	512	ASN
1	C	512	ASN
1	D	438	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	601	-	4,4,4	0.24	0	6,6,6	0.28	0
3	JSJ	A	602	-	37,42,42	2.59	9 (24%)	49,67,67	2.16	15 (30%)
4	ADP	C	602	-	28,29,29	1.46	3 (10%)	43,45,45	2.27	13 (30%)
3	JSJ	B	601	-	37,42,42	2.61	9 (24%)	49,67,67	2.34	14 (28%)
2	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.22	0
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
4	ADP	D	601	-	28,29,29	1.49	3 (10%)	43,45,45	2.47	14 (32%)

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	-	-	3/17/62/62	0/4/4/4
4	ADP	C	602	-	-	7/16/32/32	0/3/3/3
3	JSJ	B	601	-	-	9/17/62/62	0/4/4/4
4	ADP	D	601	-	-	4/16/32/32	0/3/3/3

All (24) 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	C	602	ADP	C5-C4	4.87	1.47	1.39
4	D	601	ADP	C5-C4	4.83	1.47	1.39
3	B	601	JSJ	C5-C4	4.09	1.46	1.39
3	A	602	JSJ	C5-C4	3.85	1.46	1.39
4	D	601	ADP	C5-C6	3.65	1.51	1.41
4	C	602	ADP	C5-C6	3.33	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	JSJ	C5-C6	2.75	1.48	1.41
3	B	601	JSJ	C5-N7	-2.73	1.34	1.39
4	D	601	ADP	C8-N7	2.52	1.36	1.31
4	C	602	ADP	C8-N7	2.39	1.36	1.31
3	B	601	JSJ	C5-C6	2.38	1.47	1.41
3	A	602	JSJ	PB-O1B	-2.28	1.51	1.56
3	A	602	JSJ	C4-N9	-2.28	1.32	1.37
3	B	601	JSJ	C11-C12	2.26	1.35	1.32
3	A	602	JSJ	C8-N9	-2.22	1.33	1.37
3	B	601	JSJ	C4-N9	-2.18	1.33	1.37
3	B	601	JSJ	PB-O2B	2.16	1.51	1.46
3	A	602	JSJ	C5-N7	-2.11	1.35	1.39
3	B	601	JSJ	PB-O1B	-2.08	1.51	1.56
3	A	602	JSJ	C8-N7	2.06	1.35	1.31

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	ADP	C5-C4-N3	-7.59	116.26	126.72
4	C	602	ADP	C5-C4-N3	-7.08	116.97	126.72
3	B	601	JSJ	C17-C10-N10	6.74	117.77	110.05
3	B	601	JSJ	C5-C4-N3	-6.29	118.06	126.72
3	A	602	JSJ	C5-C4-N3	-5.60	119.00	126.72
4	D	601	ADP	N3-C4-N9	5.58	136.65	127.17
4	C	602	ADP	N3-C4-N9	5.48	136.50	127.17
4	D	601	ADP	C2-N3-C4	5.13	124.36	111.83
3	A	602	JSJ	C11-C10-N10	4.93	102.82	99.43
4	D	601	ADP	C4-C5-N7	-4.92	104.96	110.58
3	B	601	JSJ	C18-C10-C11	-4.85	108.17	112.77
3	B	601	JSJ	N3-C4-N9	4.79	135.31	127.17
4	C	602	ADP	C2-N3-C4	4.68	123.25	111.83
3	A	602	JSJ	N3-C4-N9	4.49	134.81	127.17
4	D	601	ADP	N3-C2-N1	-4.30	122.07	128.58
3	B	601	JSJ	C18-C10-N10	-4.28	105.15	110.05
4	C	602	ADP	C4-C5-N7	-4.12	105.87	110.58
3	B	601	JSJ	C2-N3-C4	4.03	121.67	111.83
3	A	602	JSJ	C2-N3-C4	3.95	121.47	111.83
3	A	602	JSJ	C4-C5-N7	-3.94	106.08	110.58
4	C	602	ADP	N3-C2-N1	-3.84	122.76	128.58
3	A	602	JSJ	C4-N9-C8	3.83	109.76	105.74
4	D	601	ADP	C5-N7-C8	3.68	109.24	103.45
4	D	601	ADP	C5'-C4'-C3'	-3.65	102.06	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	ADP	C6-C5-N7	3.53	138.89	132.09
3	A	602	JSJ	C2'-C1'-N9	-3.51	104.58	113.30
3	B	601	JSJ	C11-C10-N10	3.50	101.84	99.43
3	A	602	JSJ	N3-C2-N1	-3.49	123.30	128.58
3	B	601	JSJ	N3-C2-N1	-3.36	123.50	128.58
3	B	601	JSJ	C4-C5-N7	-3.27	106.85	110.58
3	A	602	JSJ	C17-C10-C11	-3.15	109.78	112.77
4	C	602	ADP	C3'-C2'-C1'	3.12	107.37	101.46
4	C	602	ADP	C5-N7-C8	3.09	108.31	103.45
4	C	602	ADP	C5'-C4'-C3'	-3.04	104.27	115.21
3	B	601	JSJ	C17-C10-C11	2.99	115.60	112.77
3	A	602	JSJ	C5-N7-C8	2.97	108.12	103.45
3	A	602	JSJ	C6-C5-N7	2.91	137.70	132.09
3	A	602	JSJ	N9-C8-N7	-2.87	109.86	113.94
4	D	601	ADP	C3'-C2'-C1'	2.73	106.63	101.46
4	C	602	ADP	C6-C5-N7	2.71	137.31	132.09
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
4	D	601	ADP	O4'-C1'-N9	2.44	112.77	108.09
4	C	602	ADP	C4-N9-C8	2.38	108.23	105.74
4	D	601	ADP	N9-C8-N7	-2.35	110.60	113.94
3	A	602	JSJ	O1B-PB-O3A	-2.34	100.94	107.27
4	D	601	ADP	C4-N9-C8	2.26	108.11	105.74
4	C	602	ADP	O2A-PA-O1A	2.24	122.87	112.44
3	B	601	JSJ	C5-N7-C8	2.18	106.88	103.45
3	B	601	JSJ	O2A-PA-O1A	2.16	122.48	112.44
4	C	602	ADP	N9-C8-N7	-2.04	111.04	113.94
3	B	601	JSJ	C6-C5-N7	2.04	136.02	132.09
4	D	601	ADP	O2B-PB-O3A	-2.02	97.86	104.64

There are no chirality outliers.

All (23) 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

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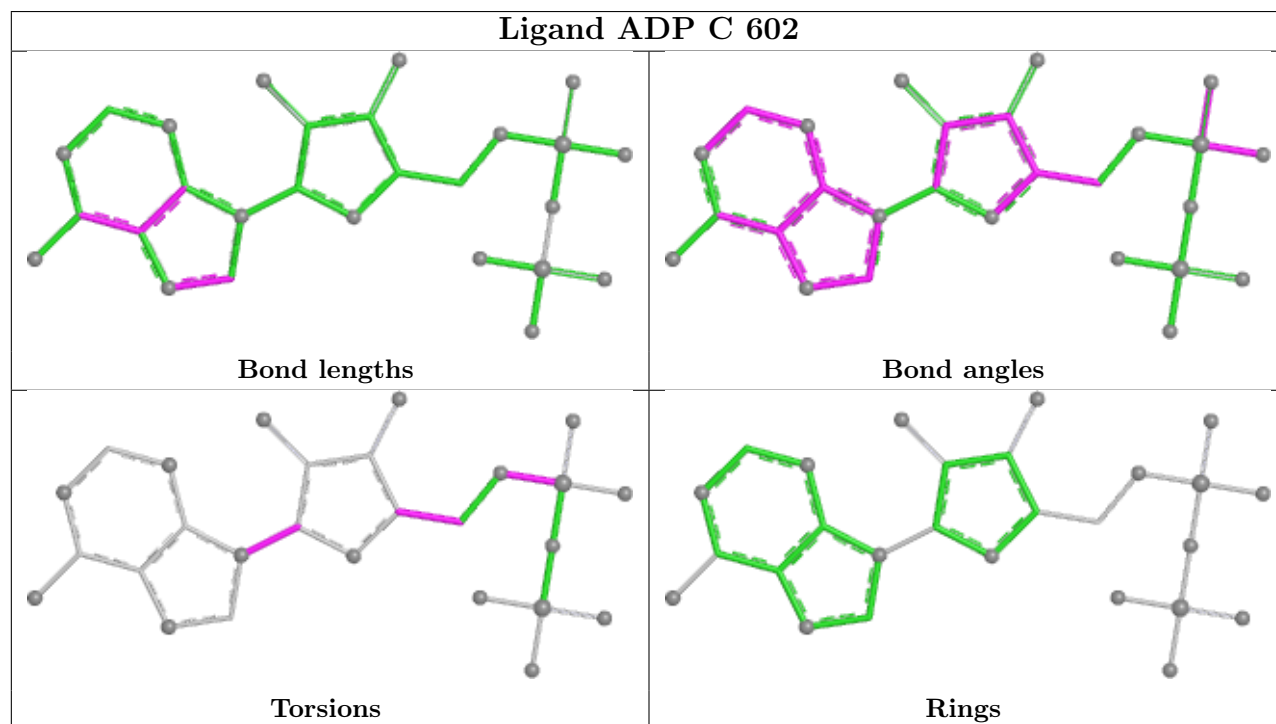
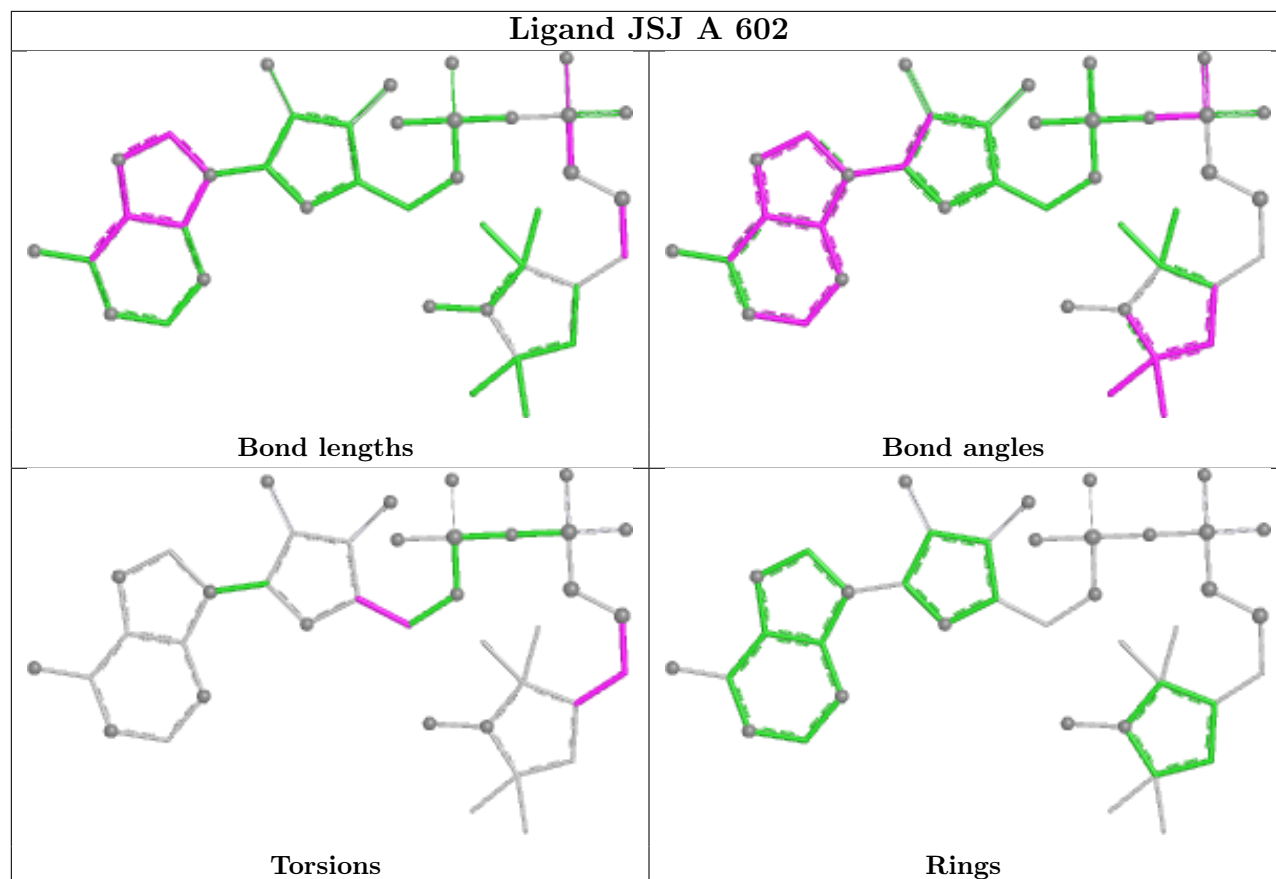
Mol	Chain	Res	Type	Atoms
4	C	602	ADP	O4'-C4'-C5'-O5'
4	D	601	ADP	C5'-O5'-PA-O2A
4	D	601	ADP	C5'-O5'-PA-O3A
4	C	602	ADP	C3'-C4'-C5'-O5'
3	B	601	JSJ	C2'-C1'-N9-C8
3	B	601	JSJ	C2'-C1'-N9-C4
4	C	602	ADP	C2'-C1'-N9-C4
3	A	602	JSJ	C11-C12-C13-S2
3	B	601	JSJ	PB-O3A-PA-O5'
3	B	601	JSJ	PA-O3A-PB-O2B
3	A	602	JSJ	C3'-C4'-C5'-O5'
4	C	602	ADP	C2'-C1'-N9-C8
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
4	D	601	ADP	C2'-C1'-N9-C8

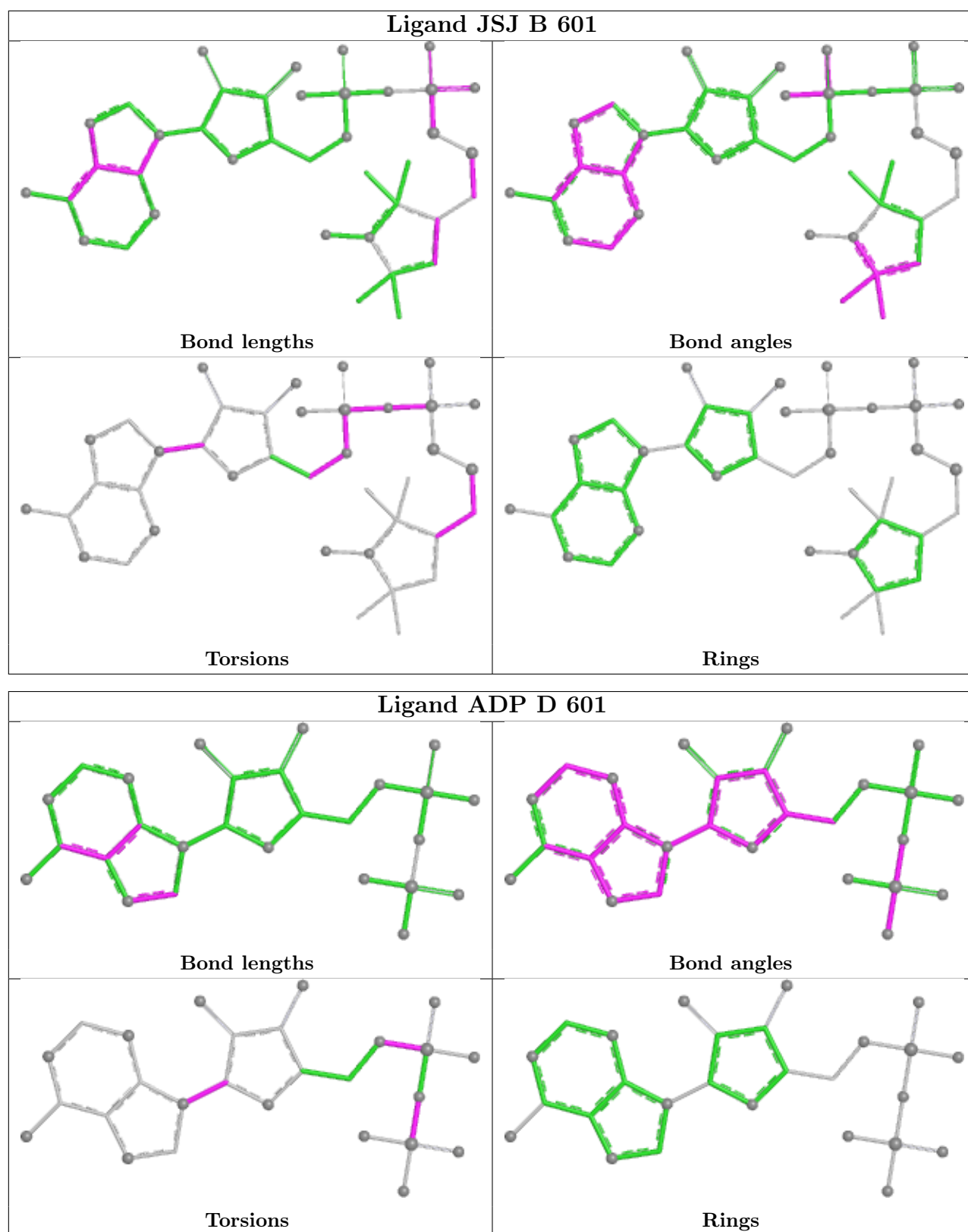
There are no ring outliers.

6 monomers are involved in 13 short contacts:

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





5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	183/187 (97%)	0.62	16 (8%) 16 14	62, 95, 132, 159	0
1	B	187/187 (100%)	0.84	21 (11%) 10 9	64, 96, 145, 185	0
1	C	184/187 (98%)	0.76	21 (11%) 10 9	67, 109, 145, 167	0
1	D	175/187 (93%)	0.70	18 (10%) 12 11	71, 113, 163, 186	0
All	All	729/748 (97%)	0.73	76 (10%) 11 10	62, 103, 150, 186	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	GLY	6.9
1	C	451	GLY	6.0
1	C	378	LYS	6.0
1	D	400	GLY	5.3
1	A	453	GLY	5.1
1	D	422	ILE	5.0
1	A	484	ASN	4.6
1	C	394	THR	4.6
1	B	401	GLU	4.3
1	C	441	ASN	4.3
1	A	512	ASN	4.1
1	B	396	VAL	4.0
1	C	371	ASP	3.9
1	D	358	ILE	3.9
1	A	511	LYS	3.2
1	C	401	GLU	3.2
1	B	394	THR	3.2
1	B	496	LYS	3.1
1	B	488	VAL	3.0
1	B	380	VAL	3.0
1	C	510	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	442	ASN	3.0
1	A	409	ASN	3.0
1	B	508	ASP	3.0
1	D	428	PRO	2.9
1	A	457	GLU	2.9
1	B	448	GLU	2.9
1	D	478	SER	2.9
1	A	520	SER	2.8
1	C	519	GLY	2.8
1	B	413	HIS	2.8
1	B	510	VAL	2.7
1	D	514	VAL	2.7
1	A	464	ILE	2.6
1	C	376	MET	2.6
1	D	421	ARG	2.6
1	B	495	GLU	2.6
1	D	466	LYS	2.5
1	C	467	GLY	2.5
1	C	476	THR	2.5
1	A	369	VAL	2.5
1	B	440	GLY	2.4
1	A	371	ASP	2.4
1	C	486	LEU	2.4
1	C	392	ASP	2.4
1	B	360	PHE	2.3
1	C	368	MET	2.3
1	C	356	VAL	2.3
1	A	518	ASN	2.3
1	A	506	GLY	2.3
1	D	520	SER	2.3
1	D	432	LEU	2.3
1	C	461	ARG	2.3
1	B	446	GLU	2.2
1	D	474	ALA	2.2
1	C	457	GLU	2.2
1	A	356	VAL	2.2
1	D	363	ASN	2.2
1	B	504	GLY	2.2
1	D	419	GLU	2.2
1	B	386	GLY	2.2
1	D	530	GLY	2.2
1	B	520	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	428	PRO	2.1
1	D	423	ALA	2.1
1	B	376	MET	2.1
1	C	445	ILE	2.1
1	D	464	ILE	2.1
1	A	414	GLY	2.1
1	B	390	GLU	2.1
1	D	527	LYS	2.0
1	C	432	LEU	2.0
1	A	498	SER	2.0
1	C	381	ASN	2.0
1	A	463	ALA	2.0
1	D	387	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

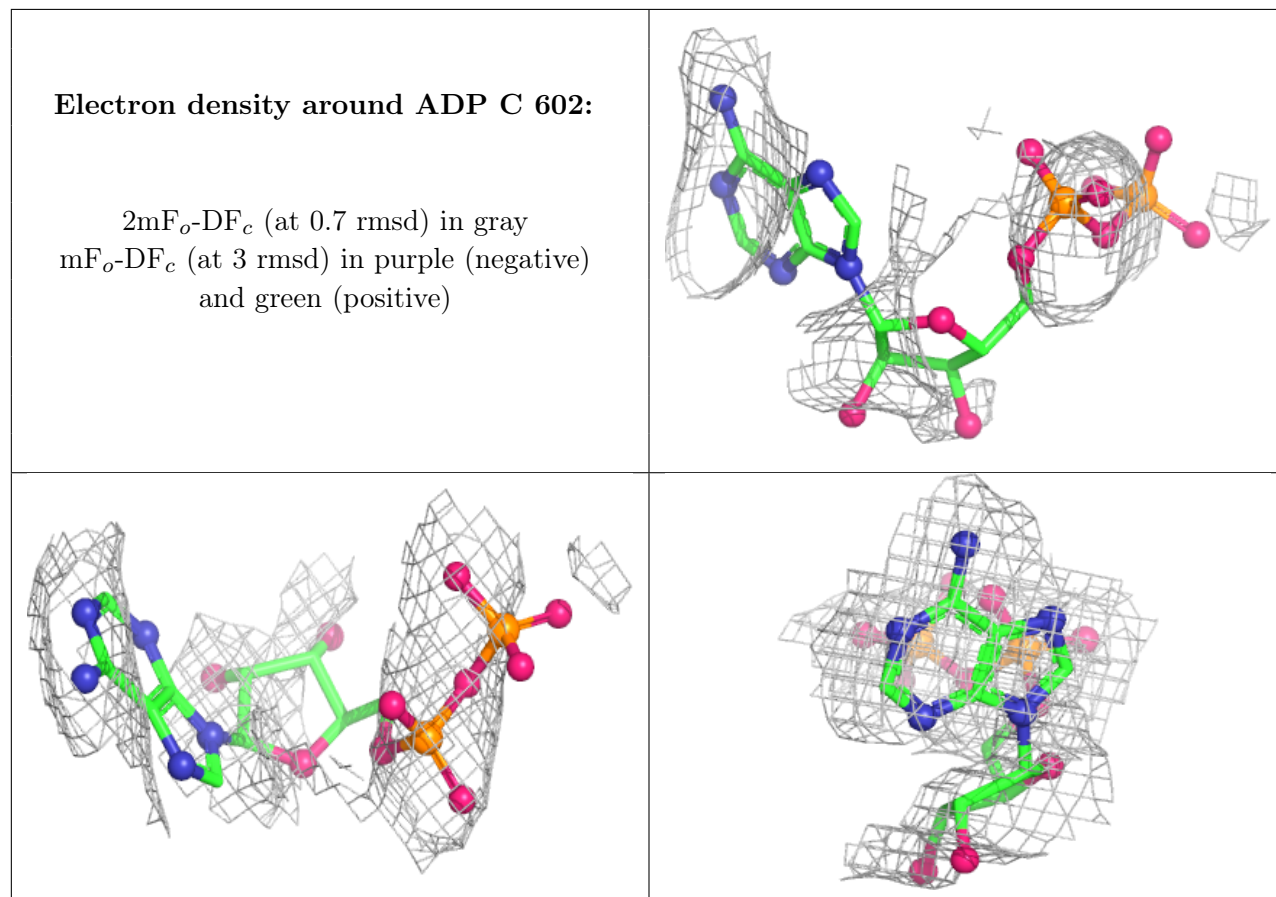
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	C	602	27/27	0.90	0.12	112,134,145,148	0
3	JSJ	A	602	39/39	0.93	0.13	84,113,180,183	0
2	SO4	C	601	5/5	0.94	0.11	95,100,101,102	0
4	ADP	D	601	27/27	0.94	0.10	99,118,126,129	0
2	SO4	A	603	5/5	0.95	0.08	94,98,110,113	0
3	JSJ	B	601	39/39	0.95	0.10	79,99,172,174	0
2	SO4	A	601	5/5	0.98	0.07	92,103,106,109	0
2	SO4	C	603	5/5	0.99	0.06	62,68,76,82	0

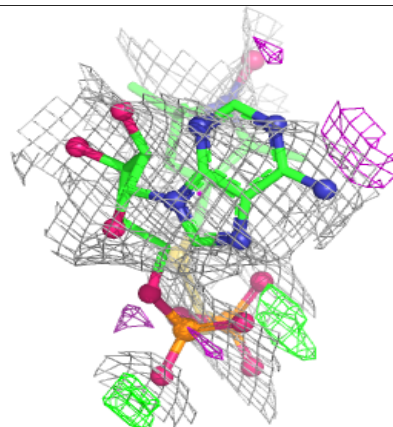
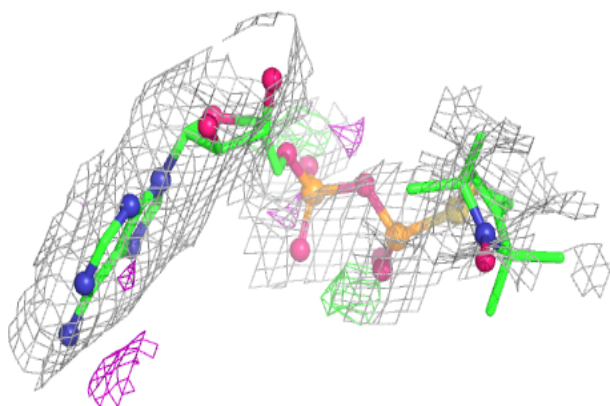
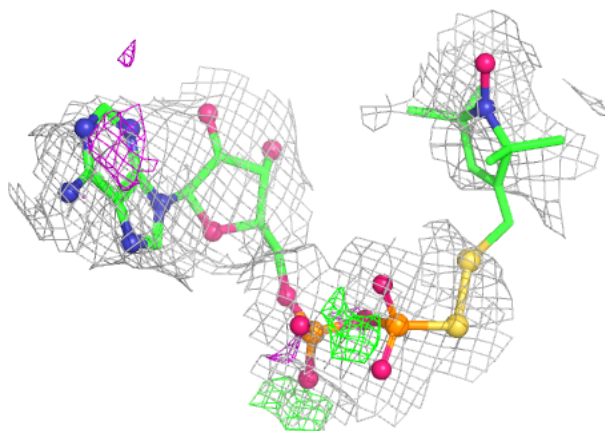
The following is a graphical depiction of the model fit to experimental electron density of all

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.



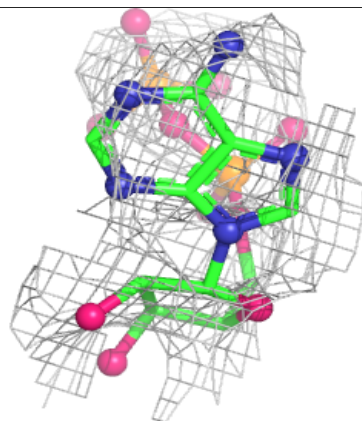
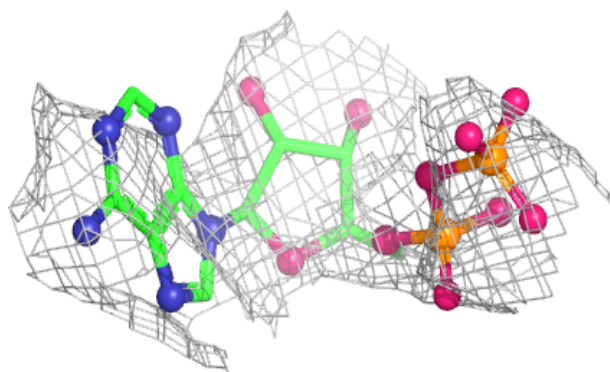
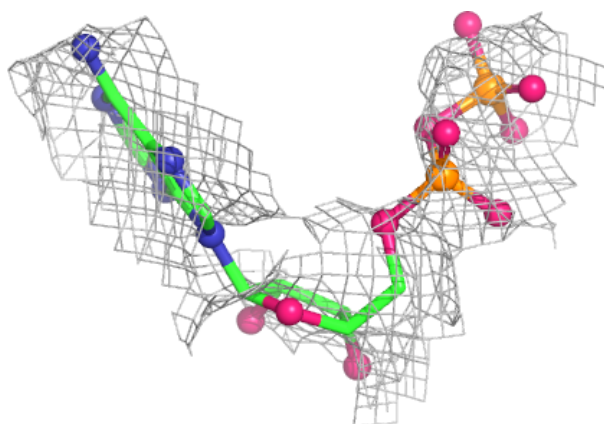
Electron density around JSJ A 602:

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



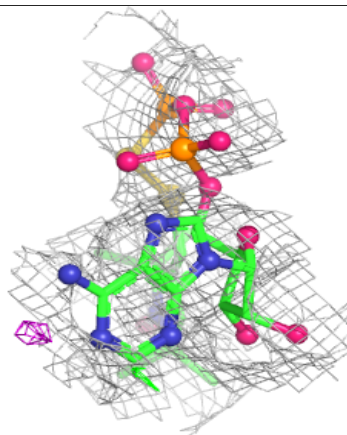
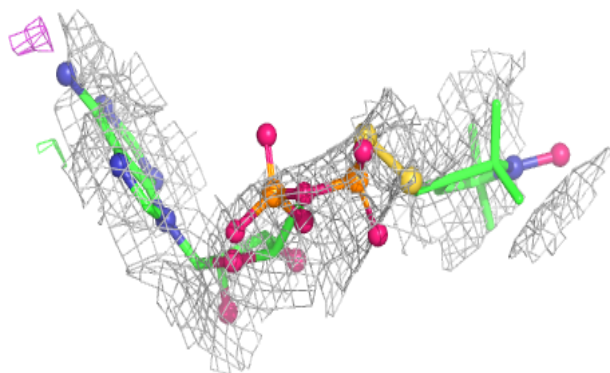
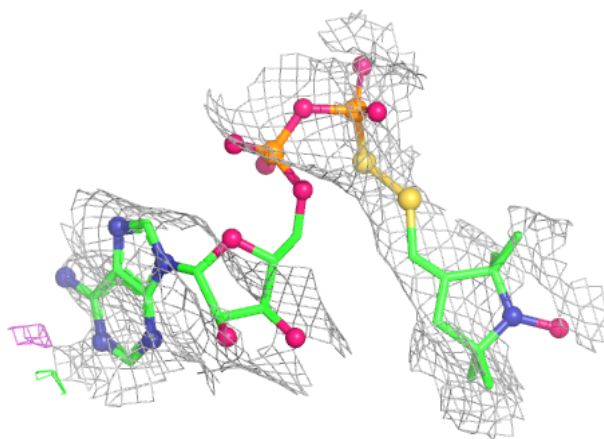
Electron density around ADP D 601:

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



Electron density around 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 [i](#)

There are no such residues in this entry.