Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 02:52 pm BST

PDB ID	:	5OFR / pdb_00005ofr
Title	:	Structure of the antibacterial peptide ABC transporter McjD in a high energy outward occluded intermediate state
Authors	:	Beis, K.; Bountra, K.
Deposited on	:	2017-07-11
Resolution	:	3.40 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:

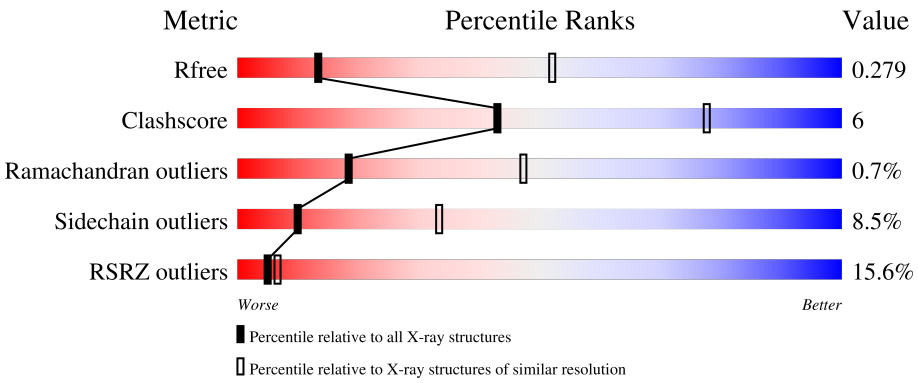
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	580	17% 76% 19% • • •
1	B	580	14% 79% 18% • •

2 Entry composition (i)

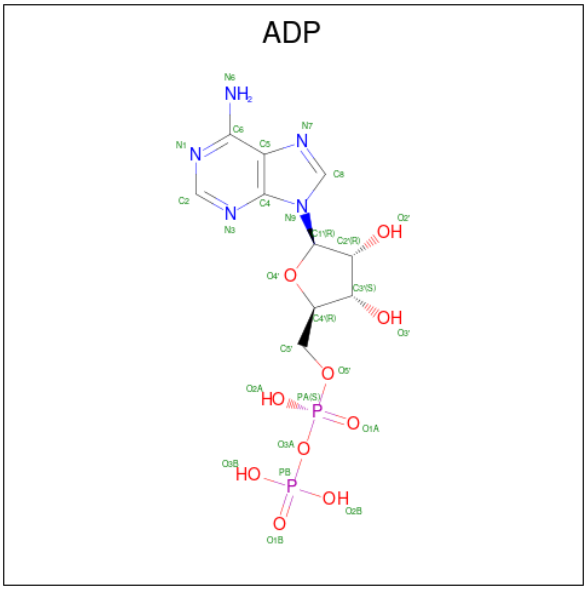
There are 4 unique types of molecules in this entry. The entry contains 9173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Microcin-J25 export ATP-binding/permease protein McjD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	571	4527	2920	739	850	18	0	0	0
1	B	576	4580	2954	750	858	18	0	2	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

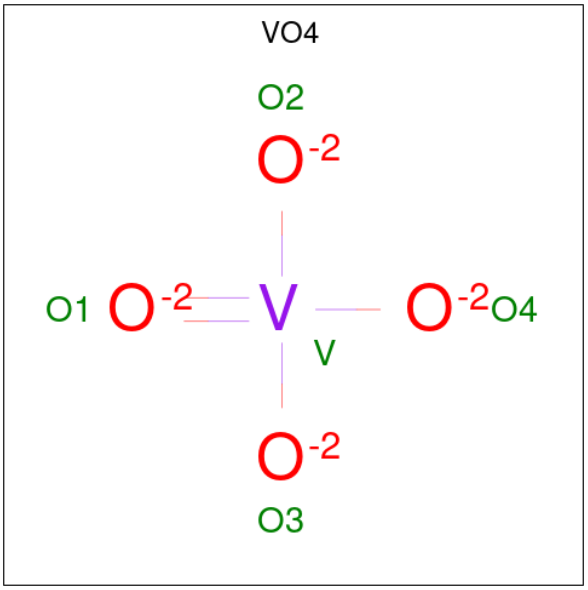


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
2	B	1	27	10	5	10	2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is VANADATE ION (CCD ID: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).



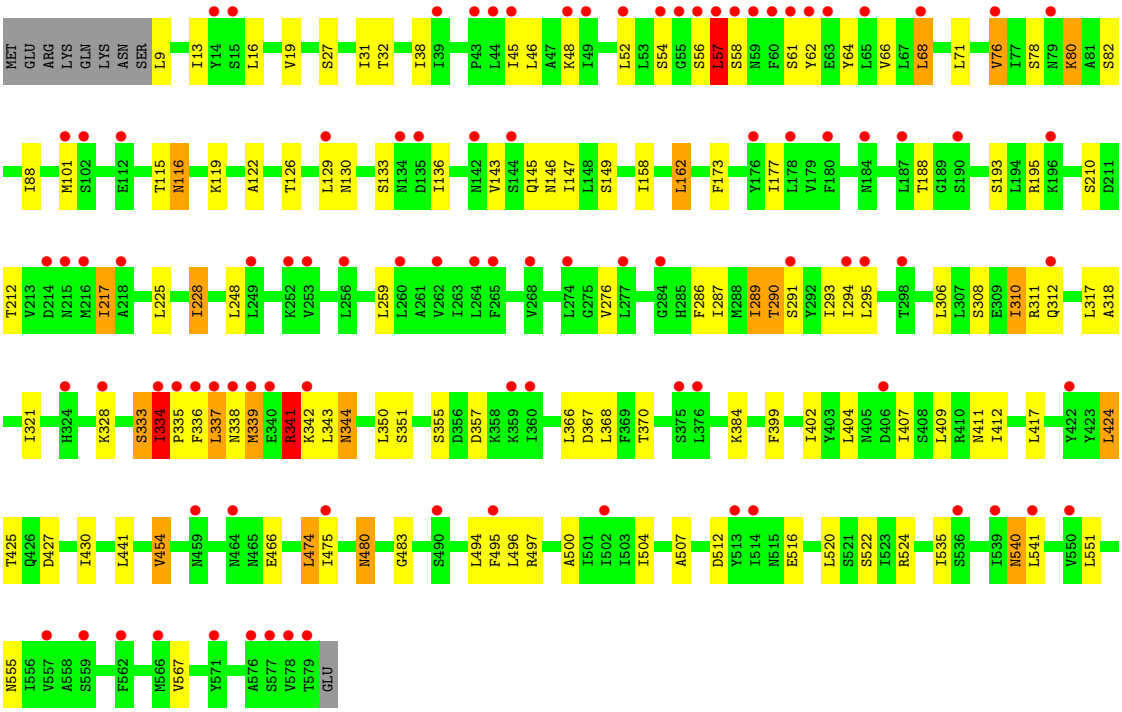
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O V 5 4 1	0	0
4	B	1	Total O V 5 4 1	0	0

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.

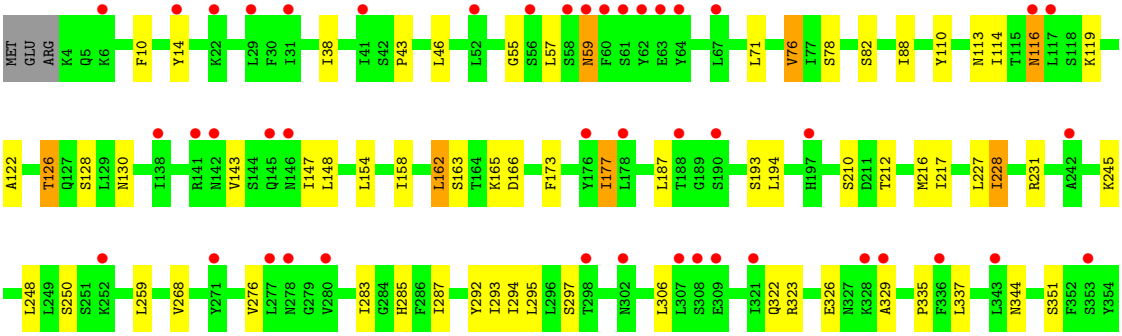
• Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD

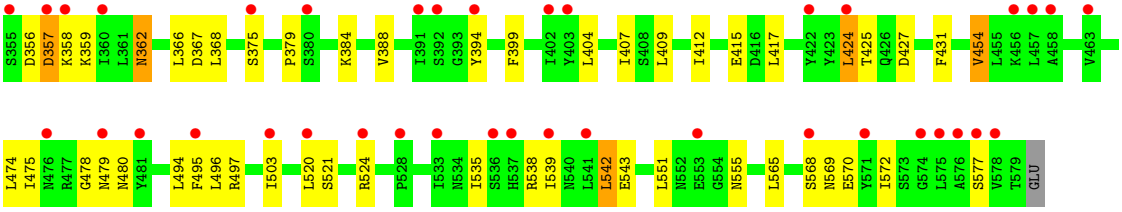
Chain A:



• Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD

Chain B:




S355 D356 D357 K358 K359 I360 L361 N362 L366 D367 L368 S375 P379 S380 K384 V388 I391 S392 G393 Y394 F399 I402 Y403 L404 I407 S408 L409 I412 E415 D416 L417 Y422 Y423 L424 T425 Q426 D427 F431 V454 L455 K456 L457 A458 V463
L474 I475 N476 R477 G478 N479 N480 Y481 L494 F495 L496 R497 I503 L520 S521 R524 P528 I533 N534 I535 S536 H537 R538 I539 N540 L541 L542 E543 L551 N552 E553 G554 N555 L565 S568 N569 E570 Y571 I572 S573 G574 L575 A576 S577 V578 T579 GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.29Å 105.04Å 117.37Å 90.00° 105.55° 90.00°	Depositor
Resolution (Å)	95.30 – 3.40 95.30 – 3.40	Depositor EDS
% Data completeness (in resolution range)	58.6 (95.30-3.40) 58.6 (95.30-3.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.257 , 0.260 0.276 , 0.279	Depositor DCC
R_{free} test set	1068 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å^2)	86.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 105.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	9173	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, VO4

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	0.91	3/4603 (0.1%)	1.41	21/6234 (0.3%)
1	B	0.86	0/4663	1.40	18/6313 (0.3%)
All	All	0.88	3/9266 (0.0%)	1.41	39/12547 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	ILE	CA-C	8.40	1.61	1.52
1	A	336	PHE	C-N	5.87	1.42	1.33
1	A	57	LEU	CA-C	5.60	1.60	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	59	ASN	CA-CB-CG	8.71	121.31	112.60
1	A	344	ASN	CA-CB-CG	6.54	119.14	112.60
1	B	216	MET	CA-C-N	6.40	128.86	120.60
1	B	216	MET	C-N-CA	6.40	128.86	120.60
1	B	538	ARG	CA-C-N	6.25	128.66	120.60
1	B	538	ARG	C-N-CA	6.25	128.66	120.60
1	B	344	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	56	SER	CA-C-N	6.20	133.39	121.54
1	A	56	SER	C-N-CA	6.20	133.39	121.54
1	A	173	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	341	ARG	CA-C-N	5.91	131.20	121.39
1	A	341	ARG	C-N-CA	5.91	131.20	121.39
1	B	173	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	479	ASN	CA-C-N	5.76	131.23	121.14
1	B	479	ASN	C-N-CA	5.76	131.23	121.14
1	B	113	ASN	CA-C-N	5.65	128.50	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	ASN	C-N-CA	5.65	128.50	120.53
1	A	540	ASN	CA-CB-CG	5.64	118.25	112.60
1	A	480	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	336	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	424	LEU	CA-C-N	5.29	128.74	120.75
1	B	424	LEU	C-N-CA	5.29	128.74	120.75
1	A	441	LEU	CA-C-N	5.29	127.80	120.29
1	A	441	LEU	C-N-CA	5.29	127.80	120.29
1	B	227	LEU	CA-C-N	5.28	127.32	120.56
1	B	227	LEU	C-N-CA	5.28	127.32	120.56
1	A	483	GLY	CA-C-N	5.26	125.78	120.00
1	A	483	GLY	C-N-CA	5.26	125.78	120.00
1	A	567	VAL	CA-C-N	5.23	127.74	120.63
1	A	567	VAL	C-N-CA	5.23	127.74	120.63
1	B	542	LEU	CA-C-N	5.17	127.16	120.44
1	B	542	LEU	C-N-CA	5.17	127.16	120.44
1	A	424	LEU	CA-C-N	5.13	128.50	120.75
1	A	424	LEU	C-N-CA	5.13	128.50	120.75
1	A	541	LEU	CA-C-N	5.07	127.49	120.29
1	A	541	LEU	C-N-CA	5.07	127.49	120.29
1	A	318	ALA	CA-C-N	5.04	125.69	119.99
1	A	318	ALA	C-N-CA	5.04	125.69	119.99
1	B	357	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4527	0	4638	77	0
1	B	4580	0	4701	46	2
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	5	0	0	0	0
All	All	9173	0	9363	114	2

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 6.

All (114) 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:333:SER:HB2	1:A:411:ASN:HA	1.56	0.86
1:B:359:LYS:HD3	1:B:362:ASN:HA	1.65	0.79
1:A:339:MET:HG2	1:A:343:LEU:HD21	1.66	0.77
1:A:338:ASN:HB3	1:A:339:MET:HE3	1.67	0.76
1:A:516:GLU:O	1:A:520:LEU:HD12	1.88	0.73
1:B:143:VAL:HA	1:B:147:ILE:HD12	1.73	0.70
1:A:333:SER:CB	1:A:411:ASN:HA	2.22	0.69
1:A:339:MET:HE2	1:A:404:LEU:HB3	1.74	0.69
1:A:343:LEU:HB2	1:A:500:ALA:HB1	1.75	0.68
1:A:143:VAL:HA	1:A:147:ILE:HD12	1.75	0.68
1:A:32:THR:HG21	1:A:145:GLN:HA	1.78	0.66
1:A:306:LEU:HD12	1:A:310:ILE:HG13	1.77	0.66
1:A:188:THR:HG23	1:A:308:SER:HA	1.80	0.64
1:A:45:ILE:HG23	1:A:68:LEU:CD1	2.28	0.64
1:A:339:MET:HG2	1:A:343:LEU:CD2	2.29	0.63
1:A:116:ASN:HA	1:A:119:LYS:HD2	1.83	0.61
1:A:335:PRO:HD2	1:A:411:ASN:O	2.00	0.60
1:A:454:VAL:HG22	1:A:495:PHE:HB2	1.83	0.60
1:B:454:VAL:HG22	1:B:495:PHE:HB2	1.84	0.59
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.86	0.58
1:A:217:ILE:HD12	1:A:217:ILE:H	1.69	0.57
1:B:212:THR:HG23	1:B:231:ARG:HH21	1.69	0.57
1:A:338:ASN:HB3	1:A:339:MET:CE	2.33	0.57
1:A:424:LEU:HD11	1:A:494:LEU:HD22	1.86	0.57
1:A:430:ILE:HG21	1:A:474:LEU:HD22	1.87	0.57
1:A:45:ILE:HG23	1:A:68:LEU:HD12	1.86	0.56
1:A:475:ILE:HB	1:A:480:ASN:HB2	1.87	0.56
1:A:343:LEU:HD12	1:A:500:ALA:HB3	1.88	0.56
1:B:424:LEU:HD11	1:B:494:LEU:HD22	1.88	0.56
1:A:158:ILE:O	1:A:162:LEU:HB2	2.06	0.55
1:B:57:LEU:H	1:B:59:ASN:ND2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LYS:HD2	1:A:535:ILE:HG23	1.89	0.55
1:A:80:LYS:HE3	1:B:297:SER:HB2	1.88	0.55
1:A:366:LEU:HD23	1:A:368:LEU:HD11	1.89	0.54
1:B:569:ASN:HD22	1:B:572:ILE:H	1.55	0.54
1:B:384:LYS:HD2	1:B:535:ILE:HG23	1.89	0.54
1:B:409:LEU:HA	1:B:412:ILE:HD12	1.90	0.53
1:B:454:VAL:HG21	1:B:496:LEU:HG	1.91	0.53
1:A:308:SER:O	1:A:312:GLN:HG2	2.08	0.53
1:B:366:LEU:HD23	1:B:368:LEU:HD11	1.91	0.53
1:A:58:SER:H	1:A:61:SER:HB3	1.74	0.52
1:A:512:ASP:OD2	1:B:379:PRO:HA	2.09	0.52
1:B:375:SER:HB3	1:B:542:LEU:HD23	1.91	0.52
1:B:454:VAL:HG22	1:B:495:PHE:CB	2.39	0.52
1:A:52:LEU:O	1:A:57:LEU:HG	2.10	0.51
1:A:339:MET:HE2	1:A:404:LEU:CB	2.39	0.51
1:B:475:ILE:HB	1:B:480:ASN:HB2	1.91	0.51
1:B:116:ASN:HA	1:B:119:LYS:HD3	1.93	0.51
1:B:217:ILE:HD12	1:B:217:ILE:H	1.76	0.51
1:A:146:ASN:O	1:A:306:LEU:HD22	2.13	0.49
1:A:32:THR:HG22	1:A:149:SER:HB2	1.94	0.49
1:B:268:VAL:HG12	1:B:293:ILE:HD11	1.94	0.49
1:A:76:VAL:HG11	1:B:294:ILE:HG12	1.94	0.49
1:A:45:ILE:HG23	1:A:68:LEU:HD13	1.93	0.48
1:A:338:ASN:ND2	1:A:412:ILE:HG23	2.28	0.48
1:B:158:ILE:O	1:B:162:LEU:HB2	2.14	0.48
1:A:286:PHE:O	1:A:290:THR:HG23	2.14	0.48
1:B:565:LEU:HA	1:B:568:SER:OG	2.14	0.48
1:A:290:THR:HA	1:A:293:ILE:HD12	1.96	0.47
1:B:351:SER:HB2	1:B:399:PHE:HB2	1.95	0.47
1:A:101:MET:HE2	1:A:129:LEU:HD12	1.96	0.47
1:A:454:VAL:HG21	1:A:496:LEU:HG	1.97	0.47
1:A:58:SER:N	1:A:61:SER:HB3	2.30	0.47
1:A:339:MET:HG2	1:A:343:LEU:CG	2.45	0.46
1:A:504:ILE:HG23	1:A:507:ALA:HB3	1.97	0.46
1:B:154:LEU:HD22	1:B:177:ILE:HD13	1.96	0.46
1:A:195:ARG:HD2	1:A:312:GLN:HB2	1.96	0.46
1:A:188:THR:HG21	1:A:311:ARG:HH11	1.80	0.46
1:A:334:ILE:O	1:A:335:PRO:C	2.59	0.45
1:A:337:LEU:O	1:A:337:LEU:HG	2.16	0.45
1:B:322:GLN:O	1:B:326:GLU:HG2	2.17	0.45
1:B:194:LEU:HD22	1:B:245:LYS:HB3	1.97	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:GLY:C	1:B:480:ASN:H	2.26	0.44
1:A:46:LEU:HD12	1:A:291:SER:OG	2.17	0.44
1:A:306:LEU:CD1	1:A:310:ILE:HG13	2.46	0.44
1:A:454:VAL:HG22	1:A:495:PHE:CB	2.46	0.44
1:B:10:PHE:O	1:B:14:TYR:HD2	2.00	0.44
1:B:57:LEU:H	1:B:59:ASN:HD22	1.66	0.44
1:A:225:LEU:HB2	1:B:110:TYR:CZ	2.53	0.44
1:B:212:THR:HG22	1:B:228:ILE:HD12	2.00	0.43
1:A:122:ALA:HB1	1:B:210:SER:HB2	1.99	0.43
1:A:339:MET:HE2	1:A:404:LEU:O	2.17	0.43
1:A:339:MET:HE1	1:A:412:ILE:CD1	2.49	0.43
1:A:136:ILE:HG13	1:A:317:LEU:HD21	2.01	0.43
1:B:409:LEU:HD22	1:B:417:LEU:HD11	2.01	0.43
1:A:355:SER:C	1:A:357:ASP:H	2.27	0.43
1:A:62:TYR:CE1	1:B:283:ILE:HD11	2.55	0.42
1:A:294:ILE:HG12	1:B:76:VAL:HG11	2.02	0.42
1:A:409:LEU:HD22	1:A:417:LEU:HD11	2.00	0.42
1:A:52:LEU:HD21	1:A:64:TYR:HD2	1.85	0.42
1:A:339:MET:HE1	1:A:412:ILE:HD13	2.02	0.42
1:B:114:ILE:HD13	1:B:394:TYR:HA	2.02	0.42
1:B:163:SER:C	1:B:165:LYS:H	2.28	0.42
1:A:210:SER:HB2	1:B:122:ALA:HB1	2.01	0.42
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.87	0.41
1:B:475:ILE:H	1:B:480:ASN:HD22	1.67	0.41
1:A:350:LEU:HD22	1:A:402:ILE:HD11	2.02	0.41
1:B:166:ASP:OD2	1:B:285:HIS:HE1	2.04	0.41
1:A:317:LEU:O	1:A:321:ILE:HG12	2.21	0.41
1:B:43:PRO:HG2	1:B:292:TYR:CE1	2.56	0.41
1:A:212:THR:HG21	1:A:228:ILE:HG23	2.03	0.41
1:A:333:SER:HB2	1:A:411:ASN:CA	2.40	0.41
1:B:38:ILE:HG21	1:B:78:SER:OG	2.20	0.41
1:B:388:VAL:HB	1:B:503:ILE:HD13	2.01	0.41
1:A:27:SER:O	1:A:31:ILE:HD12	2.20	0.41
1:A:13:ILE:HA	1:A:16:LEU:HD12	2.03	0.41
1:A:38:ILE:HG21	1:A:78:SER:OG	2.21	0.40
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.98	0.40
1:A:228:ILE:HD11	1:B:431:PHE:CE2	2.57	0.40
1:A:342:LYS:HB2	1:A:370:THR:HG21	2.02	0.40
1:A:45:ILE:HD13	1:A:71:LEU:HB3	2.04	0.40
1:A:289:ILE:HD13	1:A:289:ILE:HA	1.95	0.40
1:A:351:SER:HB2	1:A:399:PHE:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ALA:O	1:B:126:THR:HB	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLY:O	1:B:55:GLY:O[2_558]	1.02	1.18
1:B:55:GLY:C	1:B:55:GLY:O[2_558]	1.99	0.21

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	569/580 (98%)	531 (93%)	33 (6%)	5 (1%)	14 42
1	B	576/580 (99%)	538 (93%)	35 (6%)	3 (0%)	24 54
All	All	1145/1160 (99%)	1069 (93%)	68 (6%)	8 (1%)	18 47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	334	ILE
1	B	335	PRO
1	A	337	LEU
1	A	341	ARG
1	B	329	ALA
1	A	333	SER
1	B	323	ARG

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	520/529 (98%)	475 (91%)	45 (9%)	9 32
1	B	527/529 (100%)	483 (92%)	44 (8%)	10 35
All	All	1047/1058 (99%)	958 (92%)	89 (8%)	10 33

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	VAL
1	A	48	LYS
1	A	54	SER
1	A	66	VAL
1	A	68	LEU
1	A	76	VAL
1	A	80	LYS
1	A	82	SER
1	A	88	ILE
1	A	115	THR
1	A	116	ASN
1	A	126	THR
1	A	130	ASN
1	A	133	SER
1	A	162	LEU
1	A	177	ILE
1	A	193	SER
1	A	217	ILE
1	A	228	ILE
1	A	248	LEU
1	A	259	LEU
1	A	276	VAL
1	A	287	ILE
1	A	289	ILE
1	A	290	THR
1	A	295	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	310	ILE
1	A	328	LYS
1	A	339	MET
1	A	341	ARG
1	A	344	ASN
1	A	367	ASP
1	A	407	ILE
1	A	425	THR
1	A	427	ASP
1	A	454	VAL
1	A	466	GLU
1	A	474	LEU
1	A	497	ARG
1	A	522	SER
1	A	524	ARG
1	A	540	ASN
1	A	551	LEU
1	A	555	ASN
1	B	71	LEU
1	B	76	VAL
1	B	82	SER
1	B	88	ILE
1	B	116	ASN
1	B	126	THR
1	B	128	SER
1	B	130	ASN
1	B	148	LEU
1	B	162	LEU
1	B	177	ILE
1	B	187	LEU
1	B	193	SER
1	B	228	ILE
1	B	248	LEU
1	B	250	SER
1	B	259	LEU
1	B	276	VAL
1	B	287	ILE
1	B	295	LEU
1	B	306	LEU
1	B	337	LEU
1	B	356	ASP
1	B	357	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	358	LYS
1	B	362	ASN
1	B	367	ASP
1	B	404	LEU
1	B	407	ILE
1	B	415	GLU
1	B	425	THR
1	B	427	ASP
1	B	454	VAL
1	B	474	LEU
1	B	497	ARG
1	B	520	LEU
1	B	521	SER
1	B	524	ARG
1	B	539	ILE
1	B	543	GLU
1	B	551	LEU
1	B	555	ASN
1	B	570	GLU
1	B	577	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	111	ASN
1	A	130	ASN
1	A	131	GLN
1	A	134	ASN
1	A	142	ASN
1	A	145	GLN
1	A	146	ASN
1	A	215	ASN
1	A	223	ASN
1	A	285	HIS
1	A	327	ASN
1	A	362	ASN
1	A	411	ASN
1	A	459	ASN
1	A	464	ASN
1	A	479	ASN
1	A	487	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	515	ASN
1	A	555	ASN
1	B	59	ASN
1	B	96	ASN
1	B	98	GLN
1	B	111	ASN
1	B	127	GLN
1	B	134	ASN
1	B	223	ASN
1	B	285	HIS
1	B	411	ASN
1	B	426	GLN
1	B	459	ASN
1	B	464	ASN
1	B	479	ASN
1	B	480	ASN
1	B	515	ASN
1	B	569	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	VO4	A	603	2,3	0,4,4	-	-	-		
2	ADP	A	601	3,4	27,29,29	0.50	0	42,45,45	0.65	1 (2%)
2	ADP	B	601	3,4	27,29,29	0.35	0	42,45,45	0.83	2 (4%)
4	VO4	B	603	2,3	0,4,4	-	-	-		

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	A	601	3,4	-	5/16/32/32	0/3/3/3
2	ADP	B	601	3,4	-	7/16/32/32	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ADP	O2B-PB-O3A	2.59	113.31	104.64
2	B	601	ADP	O3'-C3'-C2'	2.29	119.24	111.82
2	B	601	ADP	O5'-PA-O1A	2.05	117.08	109.07

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	PA-O3A-PB-O2B
2	B	601	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	C3'-C4'-C5'-O5'
2	A	601	ADP	C5'-O5'-PA-O1A
2	A	601	ADP	C5'-O5'-PA-O2A
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
2	A	601	ADP	PA-O3A-PB-O2B
2	A	601	ADP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

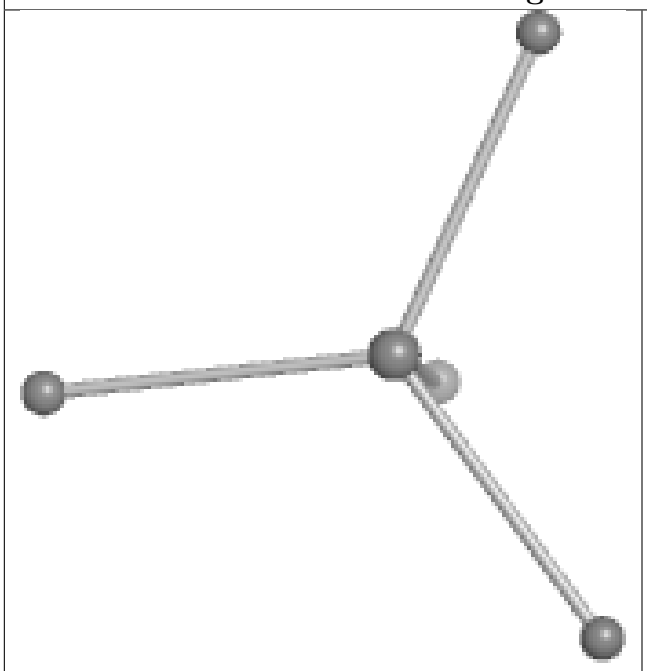
Mol	Chain	Res	Type	Atoms
2	B	601	ADP	PA-O3A-PB-O3B

There are no ring outliers.

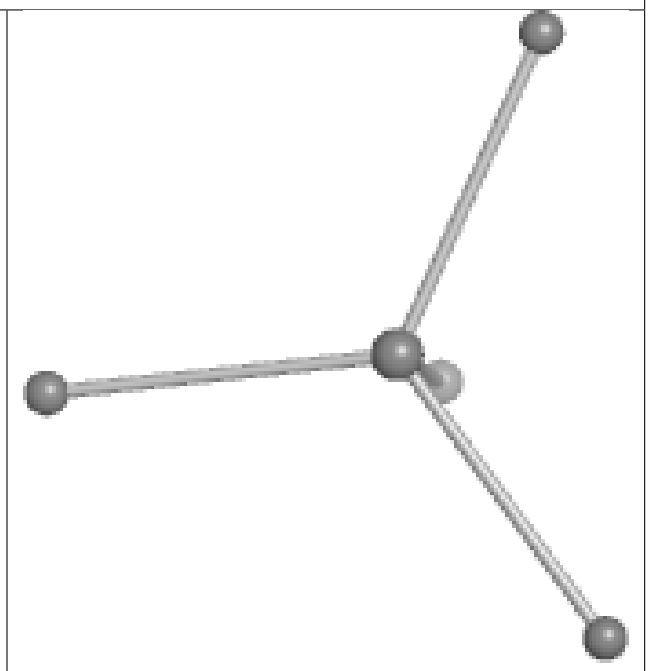
No monomer is involved in short contacts.

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.

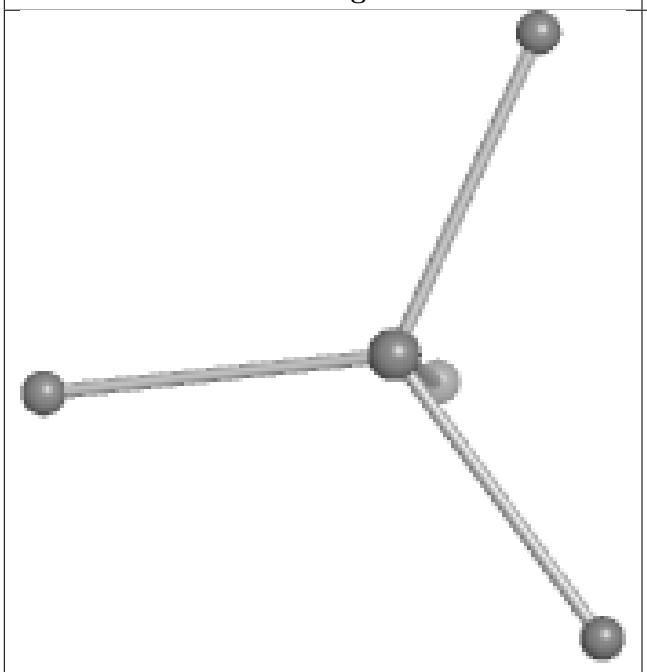
Ligand VO4 A 603



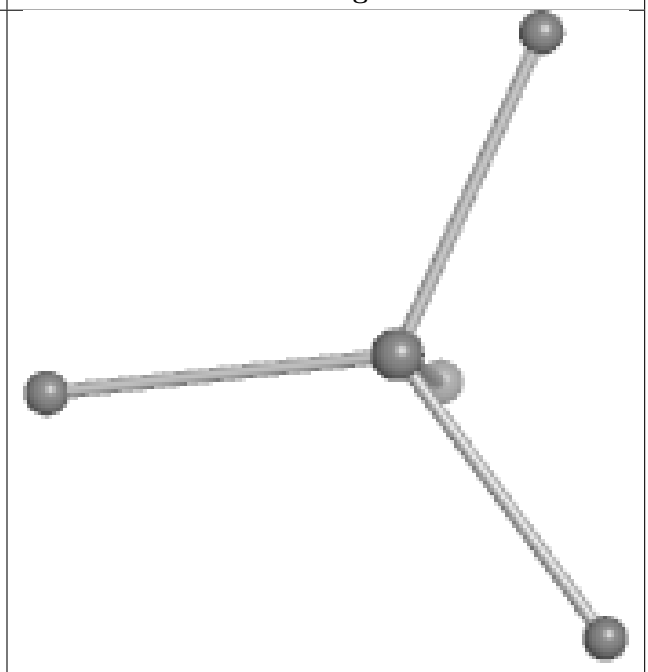
Bond lengths



Bond angles

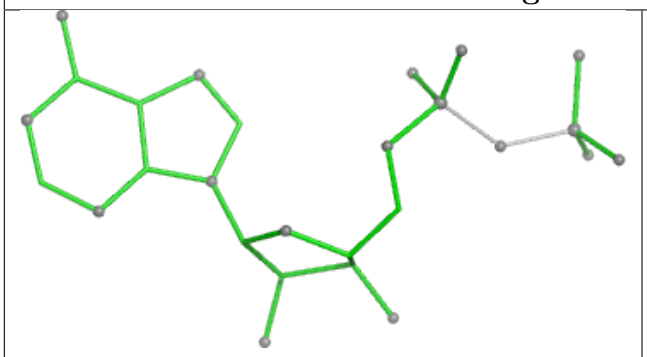


Torsions

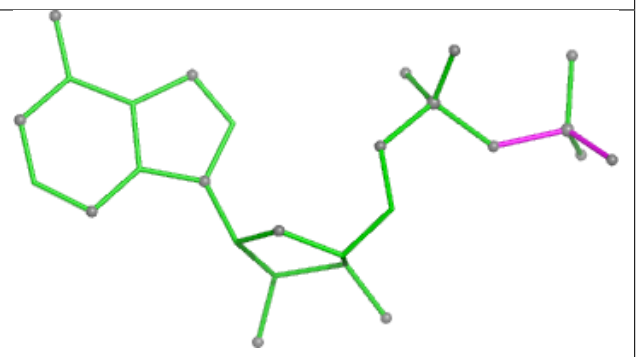


Rings

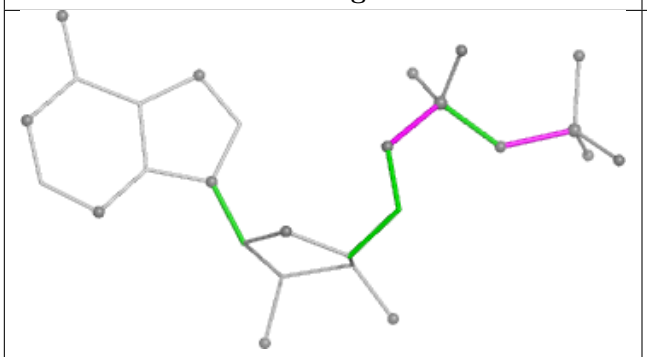
Ligand ADP A 601



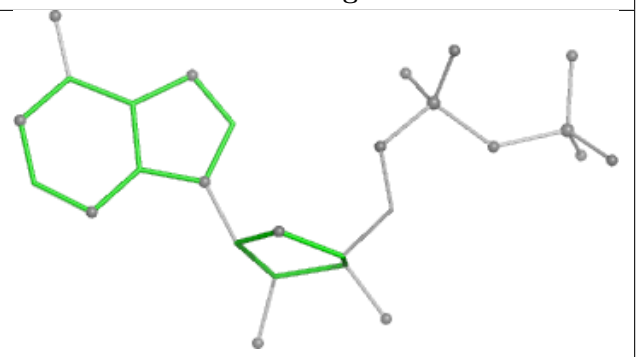
Bond lengths



Bond angles

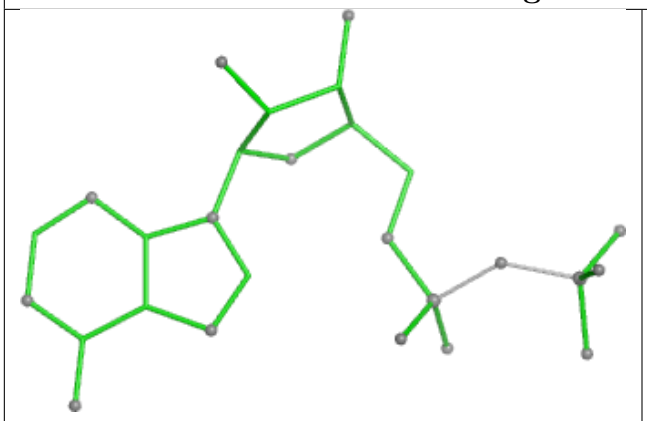


Torsions

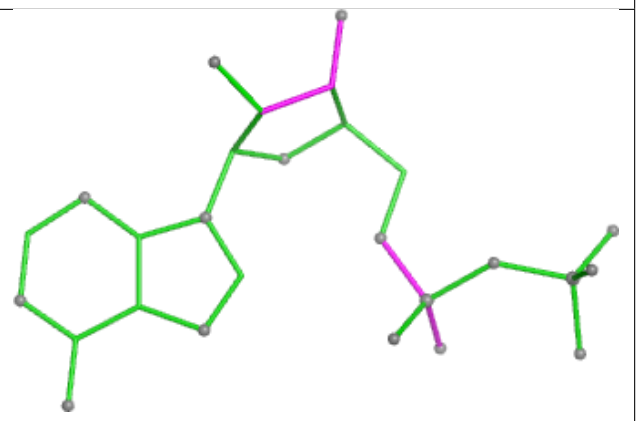


Rings

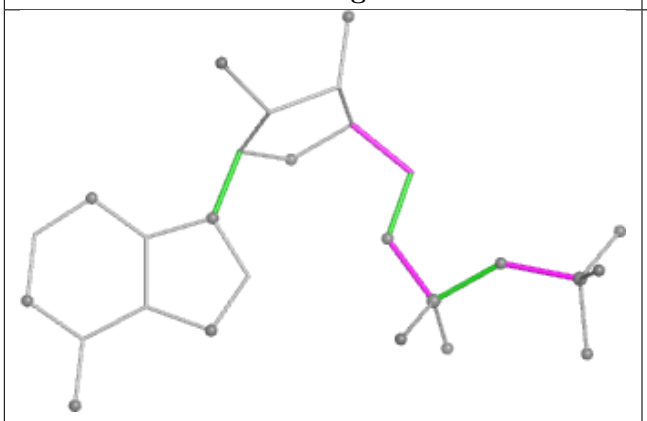
Ligand ADP B 601



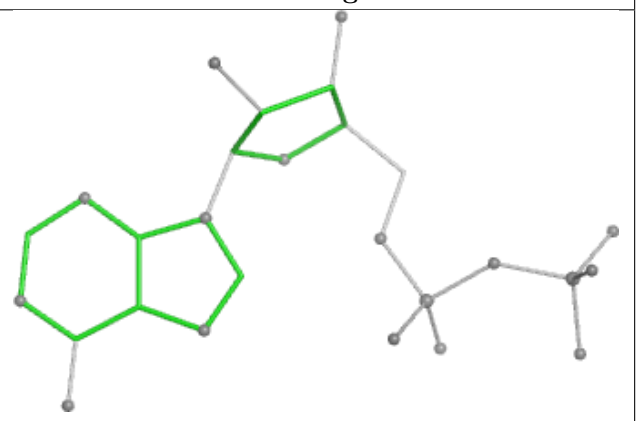
Bond lengths



Bond angles

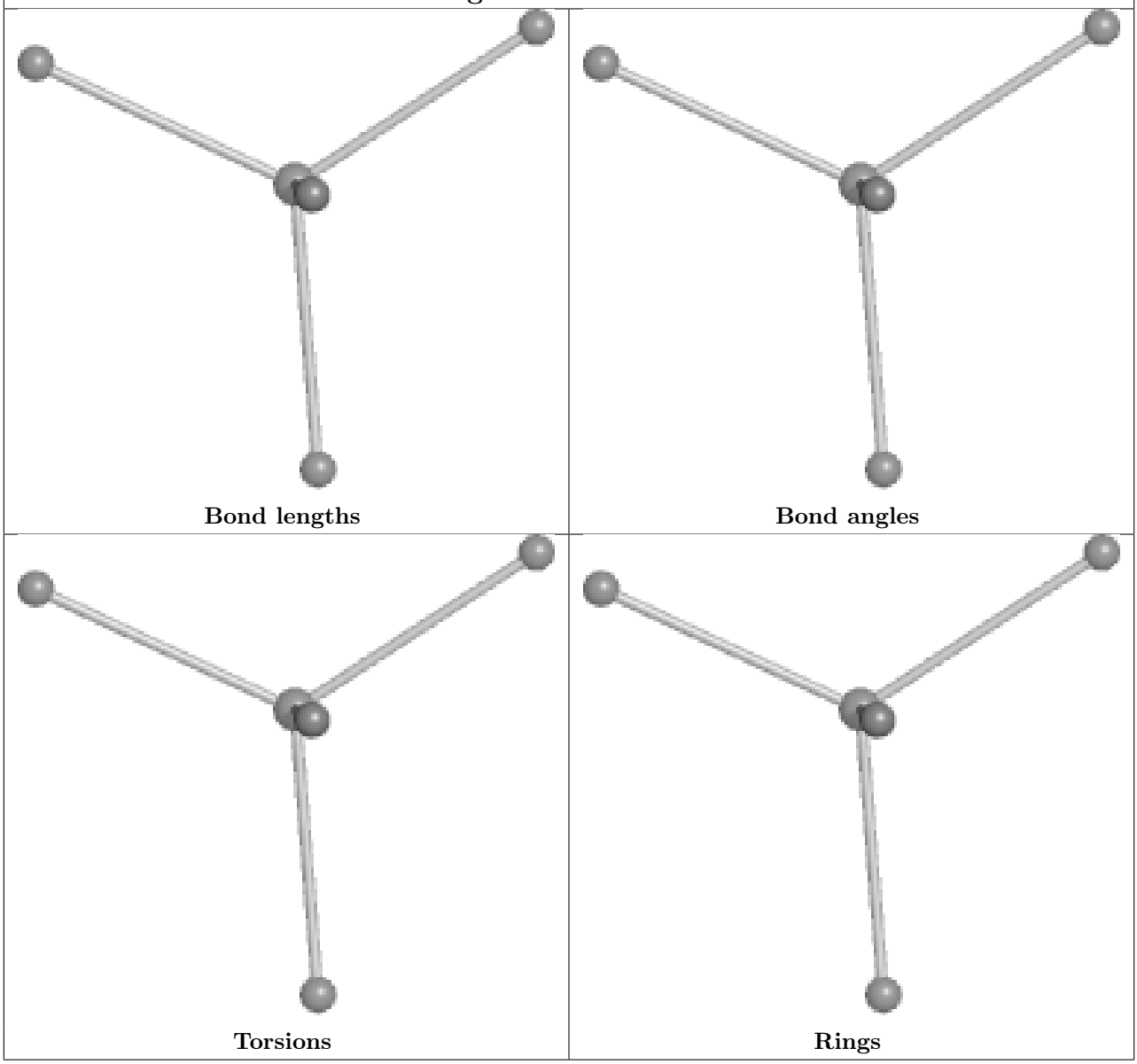


Torsions



Rings

Ligand VO4 B 603



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	571/580 (98%)	0.96	96 (16%) 4 5	47, 101, 158, 202	0
1	B	576/580 (99%)	0.99	83 (14%) 6 7	40, 109, 164, 188	2 (0%)
All	All	1147/1160 (98%)	0.98	179 (15%) 5 6	40, 106, 162, 202	2 (0%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	GLU	7.3
1	A	274	LEU	7.0
1	B	577	SER	6.0
1	B	575	LEU	5.8
1	A	295	LEU	5.8
1	B	574	GLY	5.7
1	A	291	SER	5.6
1	A	513	TYR	5.6
1	B	58	SER	5.5
1	B	357	ASP	5.3
1	A	339	MET	5.1
1	B	302	ASN	5.0
1	B	392	SER	4.8
1	A	14	TYR	4.8
1	A	79	ASN	4.8
1	B	539	ILE	4.6
1	A	44	LEU	4.5
1	A	375	SER	4.4
1	A	58	SER	4.4
1	B	578	VAL	4.3
1	A	337	LEU	4.2
1	A	56	SER	4.2
1	A	39	ILE	4.2
1	B	476	ASN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	215	ASN	4.2
1	A	57	LEU	4.1
1	B	61	SER	4.0
1	B	336	PHE	4.0
1	B	298	THR	4.0
1	A	464	ASN	4.0
1	A	101	MET	3.9
1	A	214	ASP	3.9
1	A	324	HIS	3.8
1	B	67	LEU	3.8
1	A	76	VAL	3.7
1	B	59	ASN	3.7
1	A	571	TYR	3.5
1	B	380	SER	3.5
1	B	56	SER	3.5
1	A	48	LYS	3.5
1	A	43	PRO	3.5
1	B	391	ILE	3.5
1	A	566	MET	3.5
1	A	55	GLY	3.4
1	B	458	ALA	3.4
1	B	375	SER	3.4
1	B	495	PHE	3.4
1	B	394	TYR	3.4
1	B	278	ASN	3.3
1	B	571	TYR	3.3
1	B	343	LEU	3.3
1	A	252	LYS	3.2
1	B	358	LYS	3.2
1	A	495	PHE	3.2
1	B	524	ARG	3.2
1	B	146	ASN	3.2
1	A	576	ALA	3.1
1	B	308	SER	3.1
1	B	355	SER	3.1
1	A	294	ILE	3.1
1	A	490	SER	3.1
1	B	537	HIS	3.0
1	A	360	ILE	3.0
1	A	577	SER	3.0
1	A	335	PRO	3.0
1	A	54	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	62	TYR	3.0
1	A	256	LEU	3.0
1	B	329	ALA	3.0
1	A	45	ILE	2.9
1	A	559	SER	2.9
1	B	503	ILE	2.9
1	A	578	VAL	2.9
1	B	553	GLU	2.9
1	A	334	ILE	2.9
1	B	52	LEU	2.9
1	A	65	LEU	2.9
1	B	360	ILE	2.8
1	A	190	SER	2.8
1	A	422	TYR	2.8
1	A	61	SER	2.8
1	A	60	PHE	2.8
1	B	29	LEU	2.8
1	B	141	ARG	2.8
1	B	60	PHE	2.7
1	B	252	LYS	2.7
1	B	328	LYS	2.7
1	A	539	ILE	2.7
1	B	31	ILE	2.7
1	A	52	LEU	2.7
1	B	541	LEU	2.6
1	A	268	VAL	2.6
1	A	536	SER	2.6
1	A	187	LEU	2.6
1	B	536	SER	2.6
1	B	422	TYR	2.6
1	B	528	PRO	2.6
1	A	338	ASN	2.6
1	B	353	SER	2.5
1	B	145	GLN	2.5
1	A	59	ASN	2.5
1	B	280	VAL	2.5
1	B	456	LYS	2.5
1	A	298	THR	2.5
1	B	188	THR	2.5
1	B	307	LEU	2.5
1	A	550	VAL	2.5
1	B	403	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	514	ILE	2.5
1	A	144	SER	2.5
1	B	138	ILE	2.5
1	B	309	GLU	2.5
1	B	533	ILE	2.4
1	B	576	ALA	2.4
1	A	216	MET	2.4
1	A	102	SER	2.4
1	A	49	ILE	2.4
1	A	328	LYS	2.4
1	A	376	LEU	2.4
1	A	262	VAL	2.4
1	A	359	LYS	2.3
1	B	6	LYS	2.3
1	B	14	TYR	2.3
1	B	271	TYR	2.3
1	B	402	ILE	2.3
1	A	260	LEU	2.3
1	A	562	PHE	2.3
1	A	134	ASN	2.3
1	B	142	ASN	2.3
1	A	196	LYS	2.3
1	A	284	GLY	2.3
1	A	277	LEU	2.2
1	A	176	TYR	2.2
1	B	176	TYR	2.2
1	B	321	ILE	2.2
1	A	129	LEU	2.2
1	A	264	LEU	2.2
1	B	22	LYS	2.2
1	B	62	TYR	2.2
1	A	218	ALA	2.2
1	B	197	HIS	2.2
1	A	15	SER	2.2
1	A	142	ASN	2.2
1	A	253	VAL	2.2
1	B	568	SER	2.2
1	A	63	GLU	2.2
1	A	112	GLU	2.2
1	A	579	THR	2.1
1	A	342	LYS	2.1
1	A	180	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	557	VAL	2.1
1	B	178	LEU	2.1
1	A	249	LEU	2.1
1	B	481	TYR	2.1
1	B	242	ALA	2.1
1	B	116	ASN	2.1
1	A	178	LEU	2.1
1	A	406	ASP	2.1
1	A	541	LEU	2.1
1	B	64	TYR	2.1
1	A	340	GLU	2.1
1	B	190	SER	2.1
1	B	463	VAL	2.1
1	B	479	ASN	2.1
1	B	117	LEU	2.1
1	B	277	LEU	2.1
1	B	457	LEU	2.1
1	B	520	LEU	2.1
1	A	135	ASP	2.1
1	A	312	GLN	2.1
1	A	184	ASN	2.0
1	A	502	ILE	2.0
1	B	41	ILE	2.0
1	B	424	LEU	2.0
1	A	475	ILE	2.0
1	A	459	ASN	2.0
1	A	265	PHE	2.0
1	A	336	PHE	2.0
1	A	68	LEU	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)

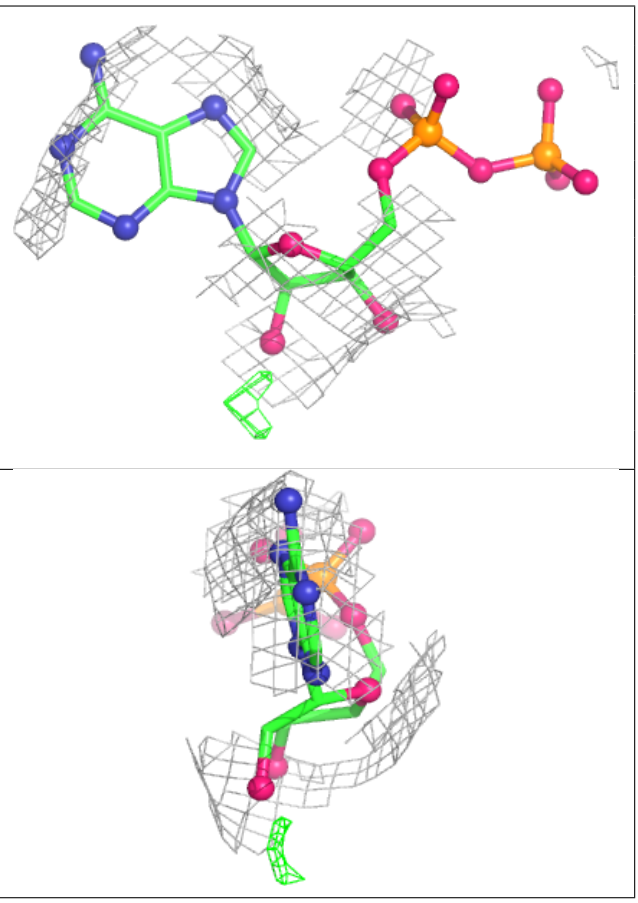
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	601	27/27	0.90	0.10	116,122,125,126	0
2	ADP	B	601	27/27	0.96	0.07	60,64,68,70	0
4	VO4	A	603	5/5	0.97	0.06	103,105,106,107	0
4	VO4	B	603	5/5	0.97	0.07	87,91,91,93	0
3	MG	B	602	1/1	0.98	0.06	37,37,37,37	0
3	MG	A	602	1/1	0.99	0.05	77,77,77,77	0

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

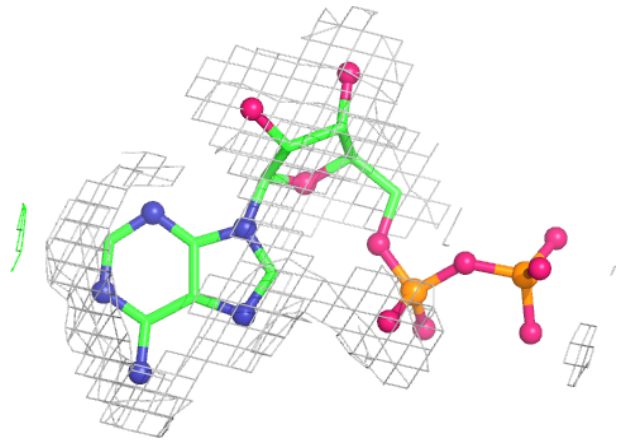
Electron density around ADP A 601:

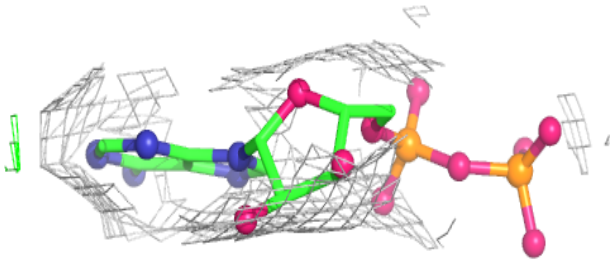
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

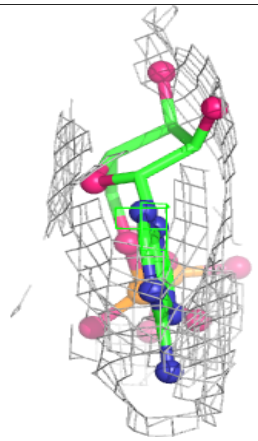


Electron density around ADP B 601:

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

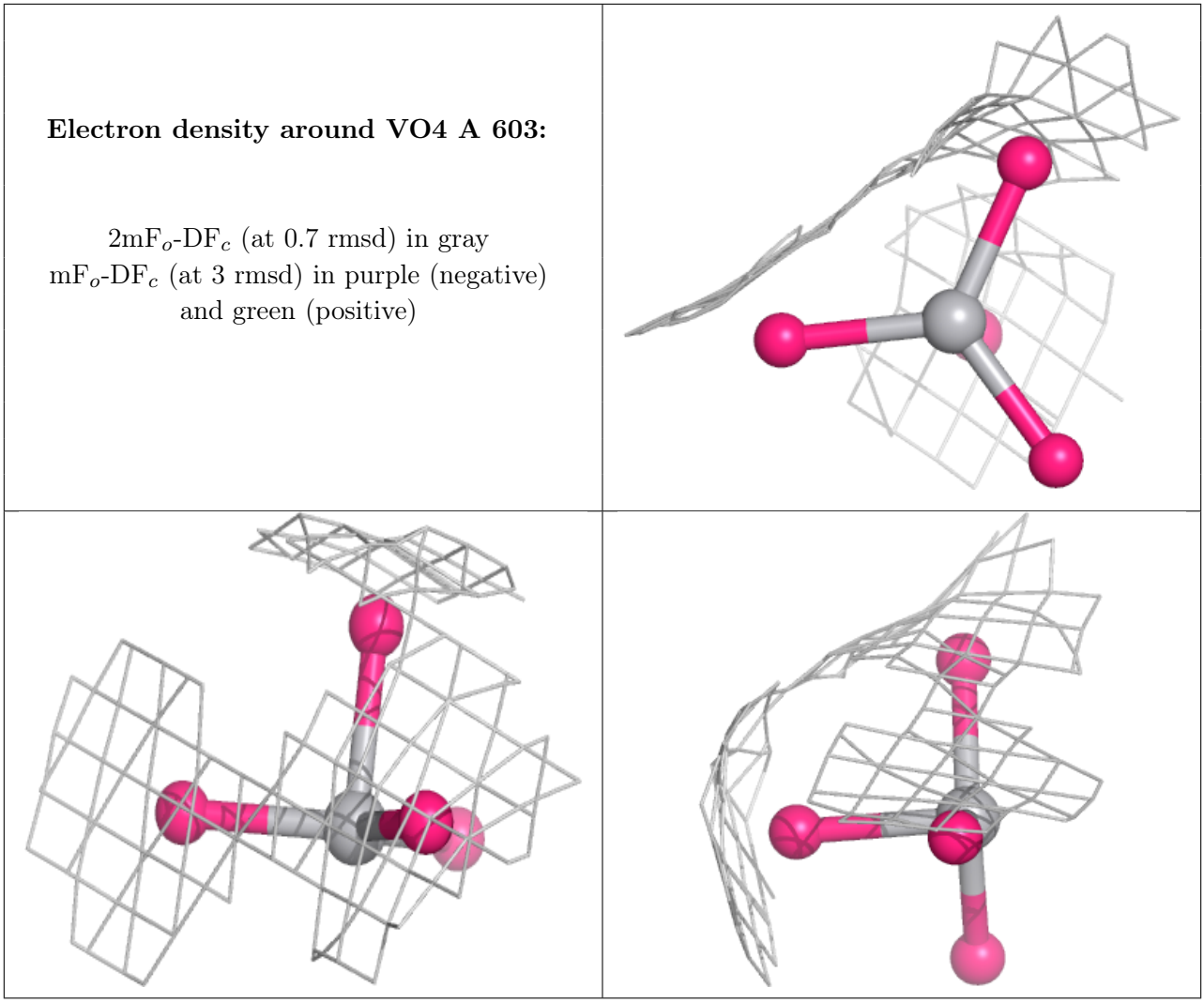






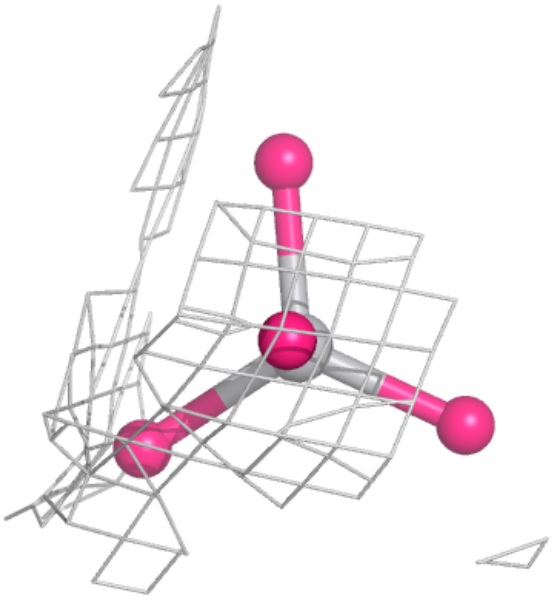
Electron density around VO4 A 603:

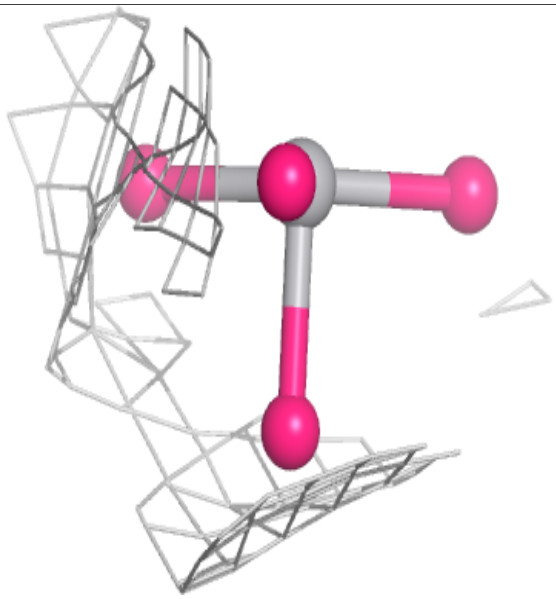
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

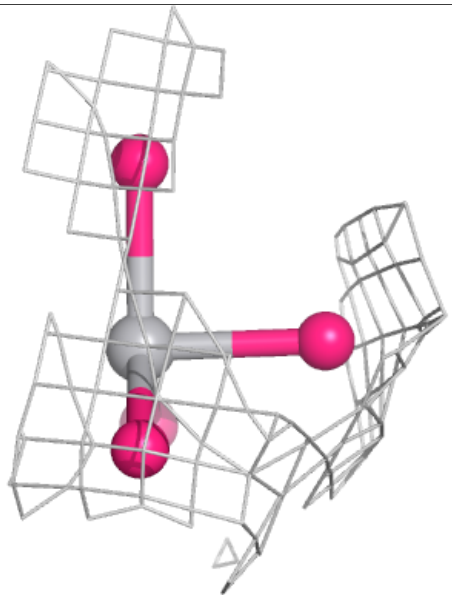


Electron density around VO4 B 603:

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

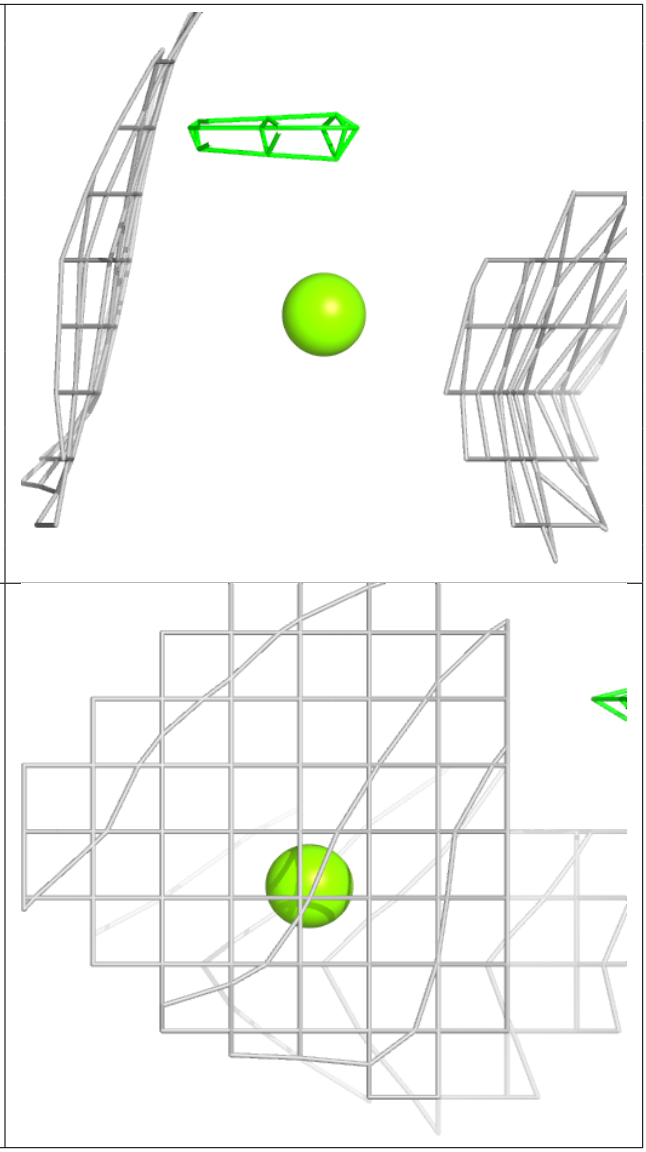






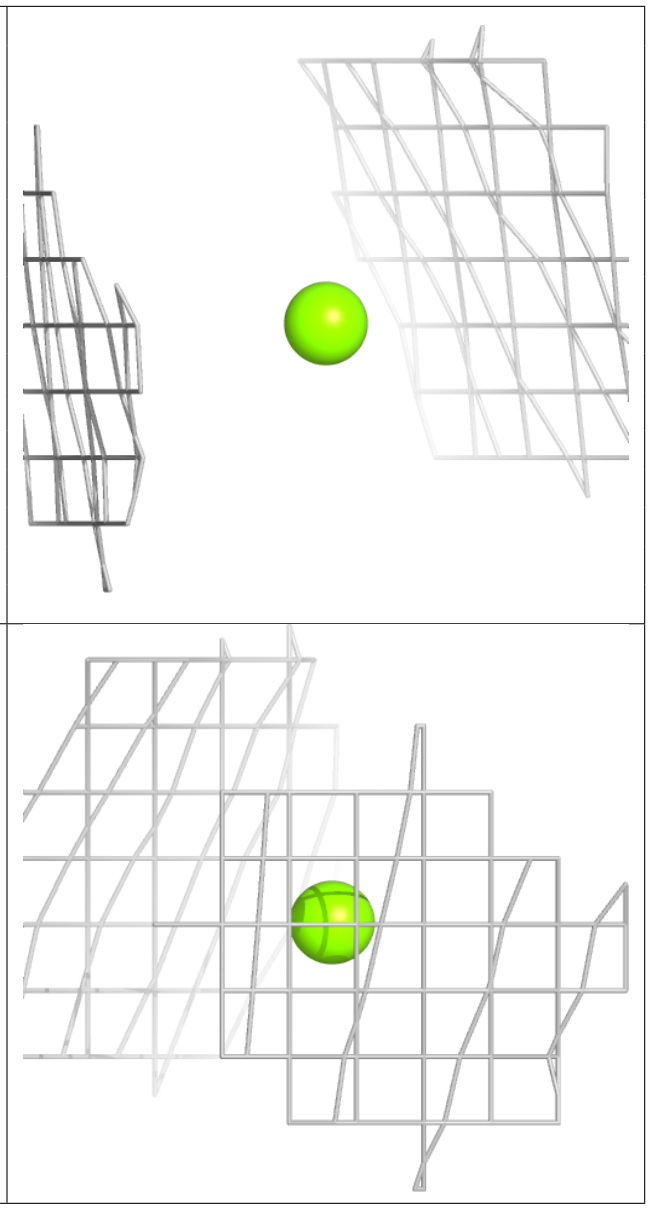
Electron density around MG B 602:

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



Electron density around MG 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)



6.5 Other polymers (i)

There are no such residues in this entry.