Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 01:44 am GMT

PDB ID	:	5OFR
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:

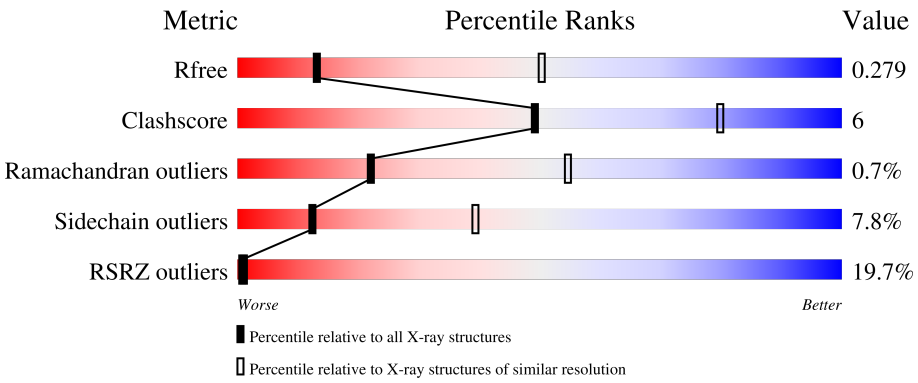
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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% 78% 18% • •
1	B	580	22% 82% 16% ••

2 Entry composition (i)

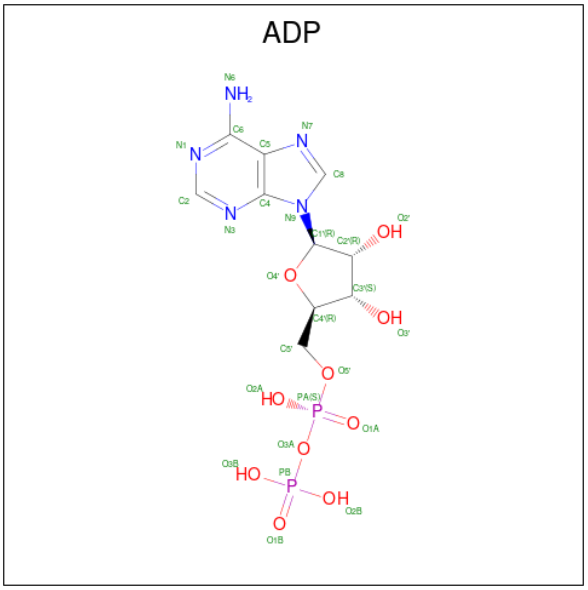
There are 4 unique types of molecules in this entry. The entry contains 9173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

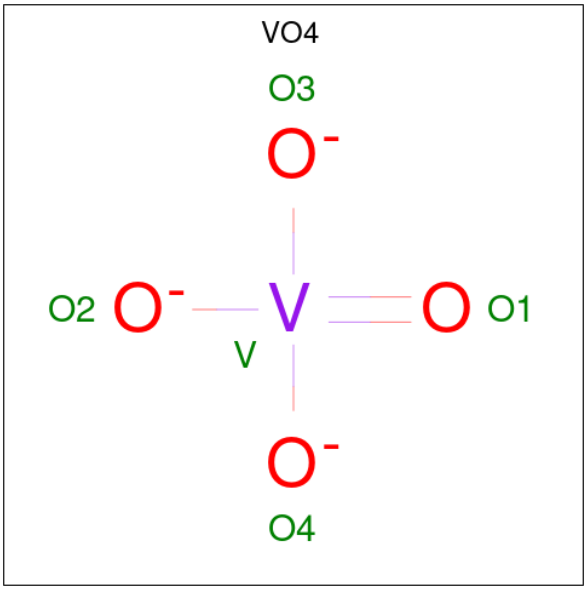


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
2	B	1	27	10	5	10	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: 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 (three-letter code: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).



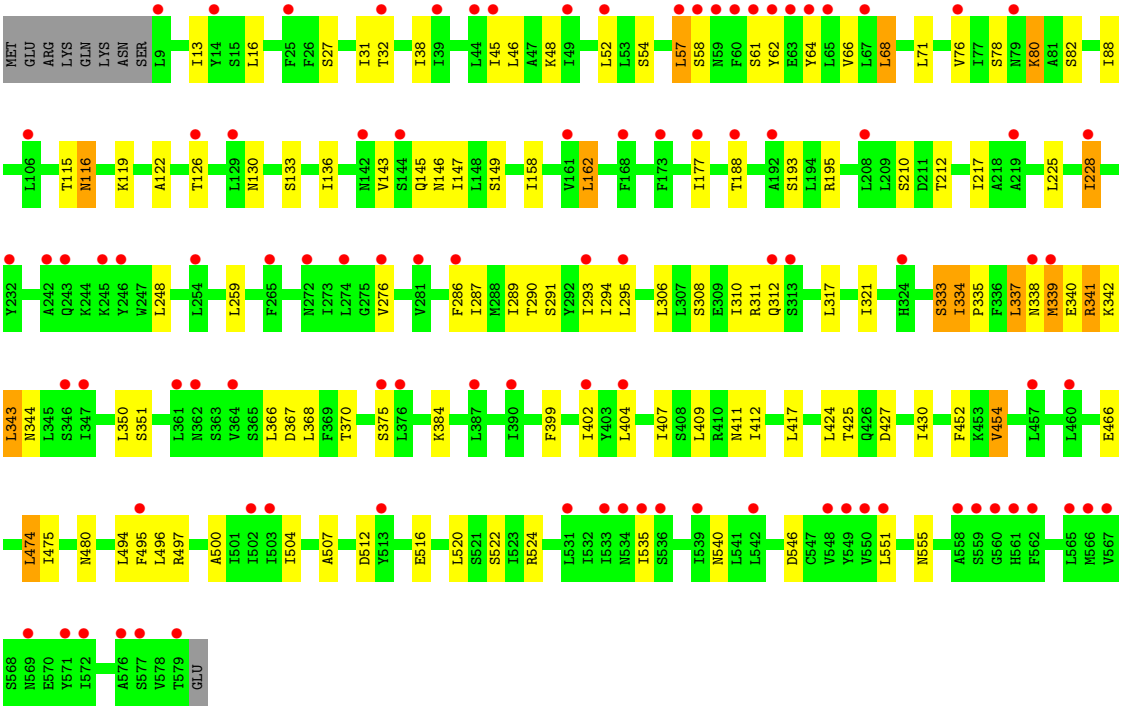
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O V 5 4 1	0	0
4	B	1	Total O V 5 4 1	0	0

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.

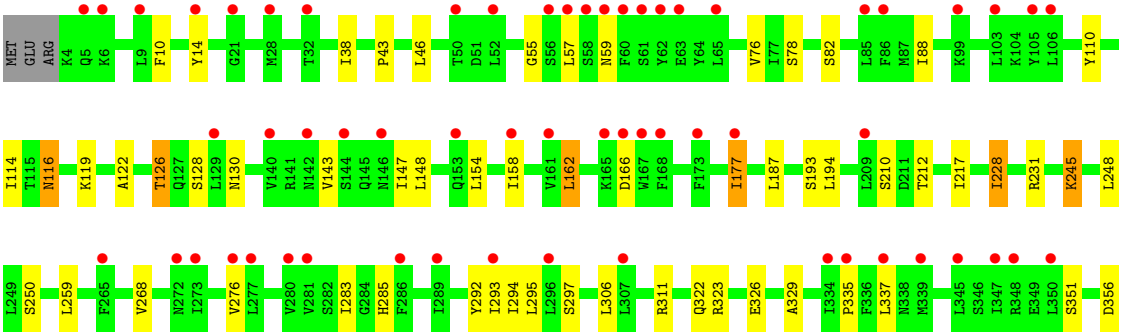
• Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD

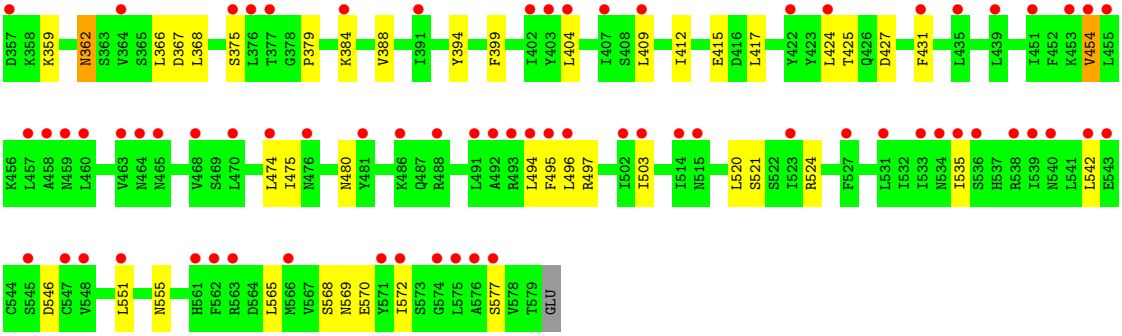
Chain A:



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

Chain B:




D357 K358 K359 N362 S363 V364 S365 L366 D367 L368 S375 L376 T377 G378 P379 K384 V388 I391 Y394 F399 I402 Y403 L404 I407 S408 L409 I412 E415 D416 L417 Y422 Y423 L424 T425 Q426 D427 F431 L435 L439 I451 F452 K453 V454 L455
K456 L457 A458 M459 L460 V463 N464 M465 V468 S469 L470 L474 I475 N476 M480 Y481 K486 Q487 R488 L491 A492 R493 L494 F495 L496 R497 I502 I503 I514 N515 L520 S521 S522 I523 R524 F527 L531 I532 I533 N534 I535 S536 H537 R538 I539 N540 L541 L542 E543
C544 S545 D546 C547 V548 L551 N555 H561 F562 R563 D564 L565 M566 V567 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 0.277 , 0.279	Depositor DCC
R_{free} test set	1068 reflections (4.78%)	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)	0.30 , 91.5	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	0.84	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: VO4, ADP, MG

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	0.52	0/4603	0.68	0/6234
1	B	0.49	0/4663	0.65	0/6313
All	All	0.51	0/9266	0.67	0/12547

There are no bond length outliers.

There are no bond angle outliers.

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	74	0
1	B	4580	0	4701	44	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
4	A	5	0	0	0	0
4	B	5	0	0	0	0
All	All	9173	0	9363	109	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 (109) 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:339:MET:HE2	1:A:404:LEU:HB3	1.66	0.76
1:A:516:GLU:O	1:A:520:LEU:HD12	1.88	0.73
1:A:338:ASN:HB3	1:A:339:MET:HE1	1.70	0.73
1:A:339:MET:HE2	1:A:404:LEU:CB	2.20	0.72
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:CB	1:A:339:MET:HE1	2.39	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: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: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:339:MET:HE2	1:A:404:LEU:HB2	1.94	0.46
1:A:188:THR:HG21	1:A:311:ARG:HH11	1.80	0.46
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
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:136:ILE:HG13	1:A:317:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD22	1:B:417:LEU:HD11	2.01	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:B:114:ILE:HD13	1:B:394:TYR:HA	2.02	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:334:ILE:O	1:A:335:PRO:C	2.59	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
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%)	17	49
1	B	576/580 (99%)	538 (93%)	35 (6%)	3 (0%)	29	61
All	All	1145/1160 (99%)	1069 (93%)	68 (6%)	8 (1%)	22	55

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%)	478 (92%)	42 (8%)	11	38
1	B	527/529 (100%)	488 (93%)	39 (7%)	13	42
All	All	1047/1058 (99%)	966 (92%)	81 (8%)	12	40

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	54	SER
1	A	66	VAL
1	A	68	LEU
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	228	ILE
1	A	248	LEU
1	A	259	LEU
1	A	276	VAL
1	A	287	ILE
1	A	295	LEU
1	A	339	MET
1	A	340	GLU
1	A	341	ARG
1	A	343	LEU
1	A	344	ASN
1	A	367	ASP
1	A	375	SER
1	A	407	ILE
1	A	425	THR
1	A	427	ASP
1	A	452	PHE
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	546	ASP
1	A	551	LEU
1	A	555	ASN
1	B	82	SER

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Mol	Chain	Res	Type
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	245	LYS
1	B	248	LEU
1	B	250	SER
1	B	259	LEU
1	B	276	VAL
1	B	295	LEU
1	B	306	LEU
1	B	311	ARG
1	B	337	LEU
1	B	356	ASP
1	B	362	ASN
1	B	367	ASP
1	B	404	LEU
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	546	ASP
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	130	ASN
1	A	153	GLN
1	A	223	ASN
1	A	464	ASN
1	A	487	GLN
1	B	59	ASN
1	B	127	GLN
1	B	130	ASN
1	B	153	GLN
1	B	362	ASN
1	B	426	GLN
1	B	459	ASN
1	B	479	ASN
1	B	480	ASN
1	B	515	ASN
1	B	555	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 monosaccharides 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	$\#\|Z\| > 2$
2	ADP	A	601	3,4	24,29,29	0.73	0	29,45,45	0.93	2 (6%)
4	VO4	A	603	3,2	1,4,4	4.90	1 (100%)	-		
2	ADP	B	601	3,4	24,29,29	0.61	0	29,45,45	1.15	4 (13%)
4	VO4	B	603	3,2	1,4,4	4.70	1 (100%)	-		

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	-	5/12/32/32	0/3/3/3
2	ADP	B	601	3,4	-	7/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	VO4	O1-V	4.90	1.91	1.63
4	B	603	VO4	O1-V	4.70	1.90	1.63

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	ADP	C3'-C2'-C1'	2.67	105.00	100.98
2	A	601	ADP	O2B-PB-O3A	2.59	113.31	104.64
2	A	601	ADP	C5-C6-N6	2.32	123.88	120.35
2	B	601	ADP	O3'-C3'-C2'	2.29	119.24	111.82
2	B	601	ADP	C5-C6-N6	2.16	123.64	120.35
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

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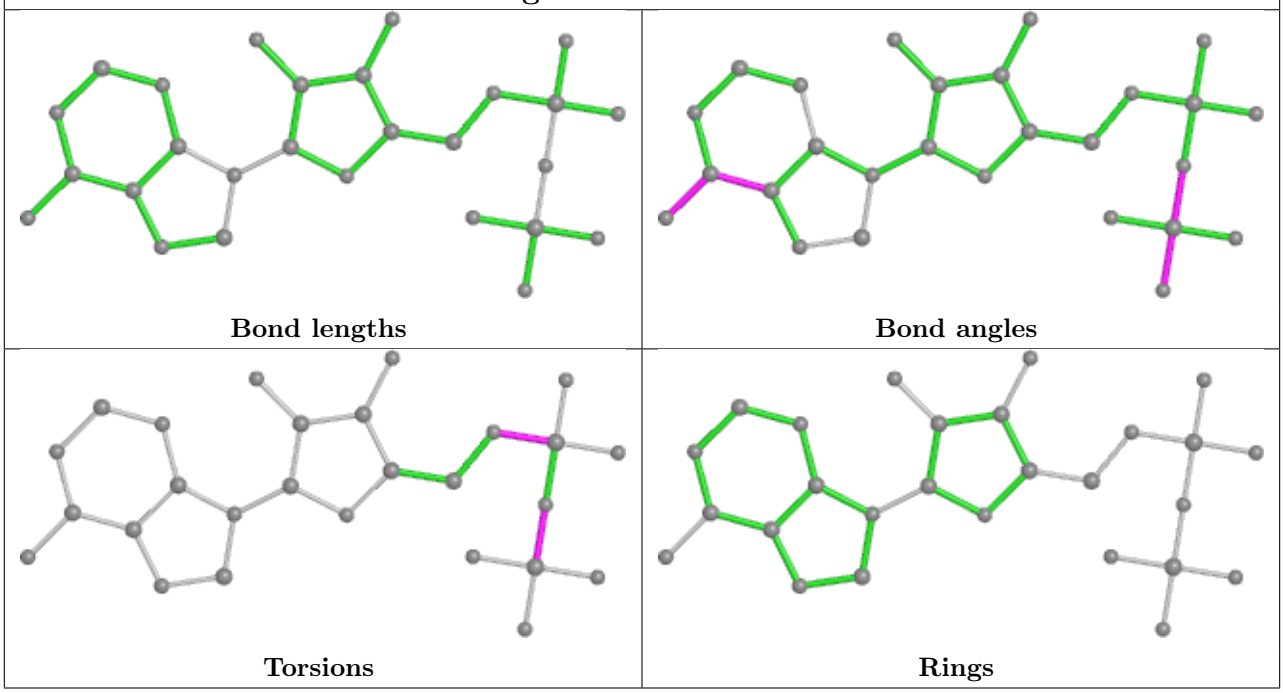
Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O2A
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
2	A	601	ADP	PA-O3A-PB-O2B
2	A	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	PA-O3A-PB-O3B

There are no ring outliers.

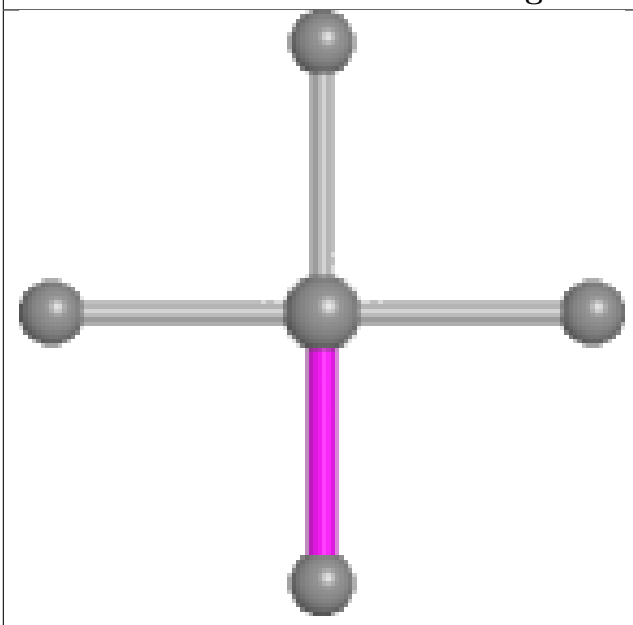
No monomer is involved in short contacts.

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.

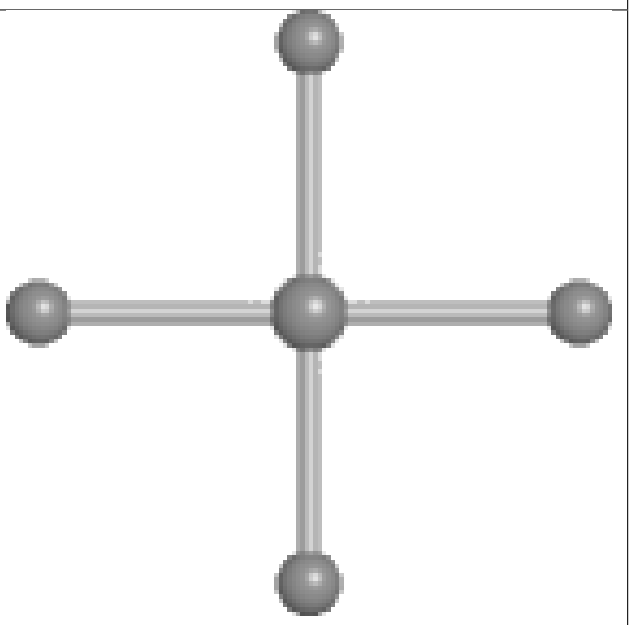
Ligand ADP A 601



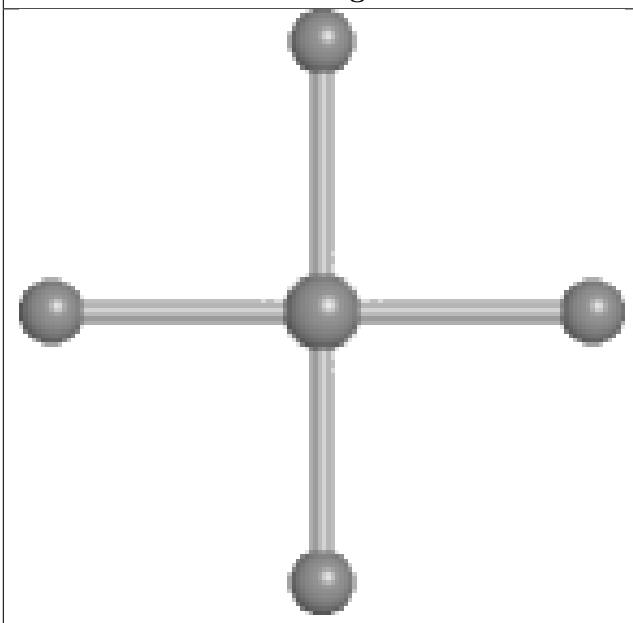
Ligand VO4 A 603



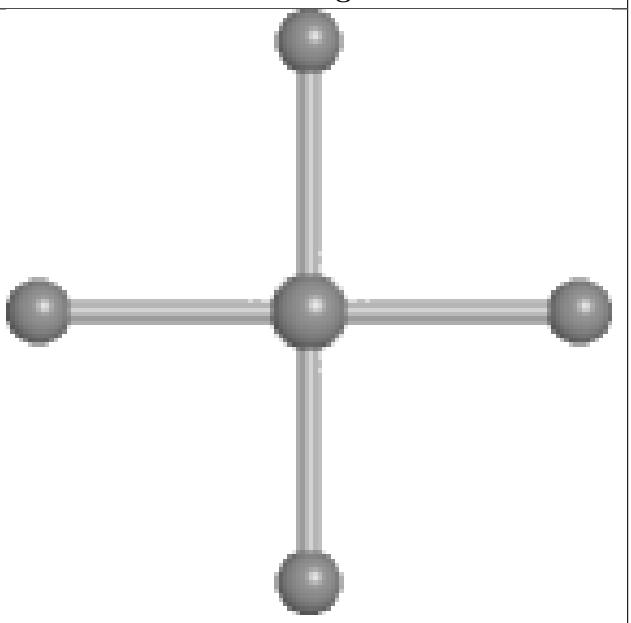
Bond lengths



Bond angles

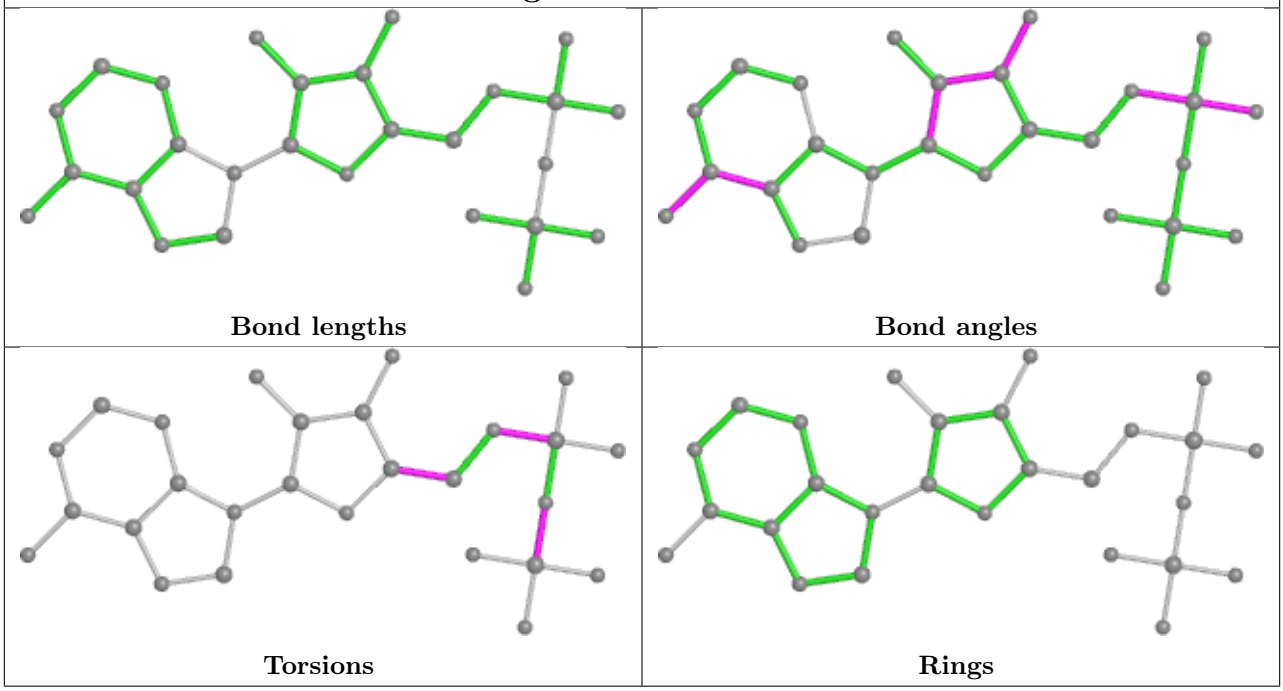


Torsions

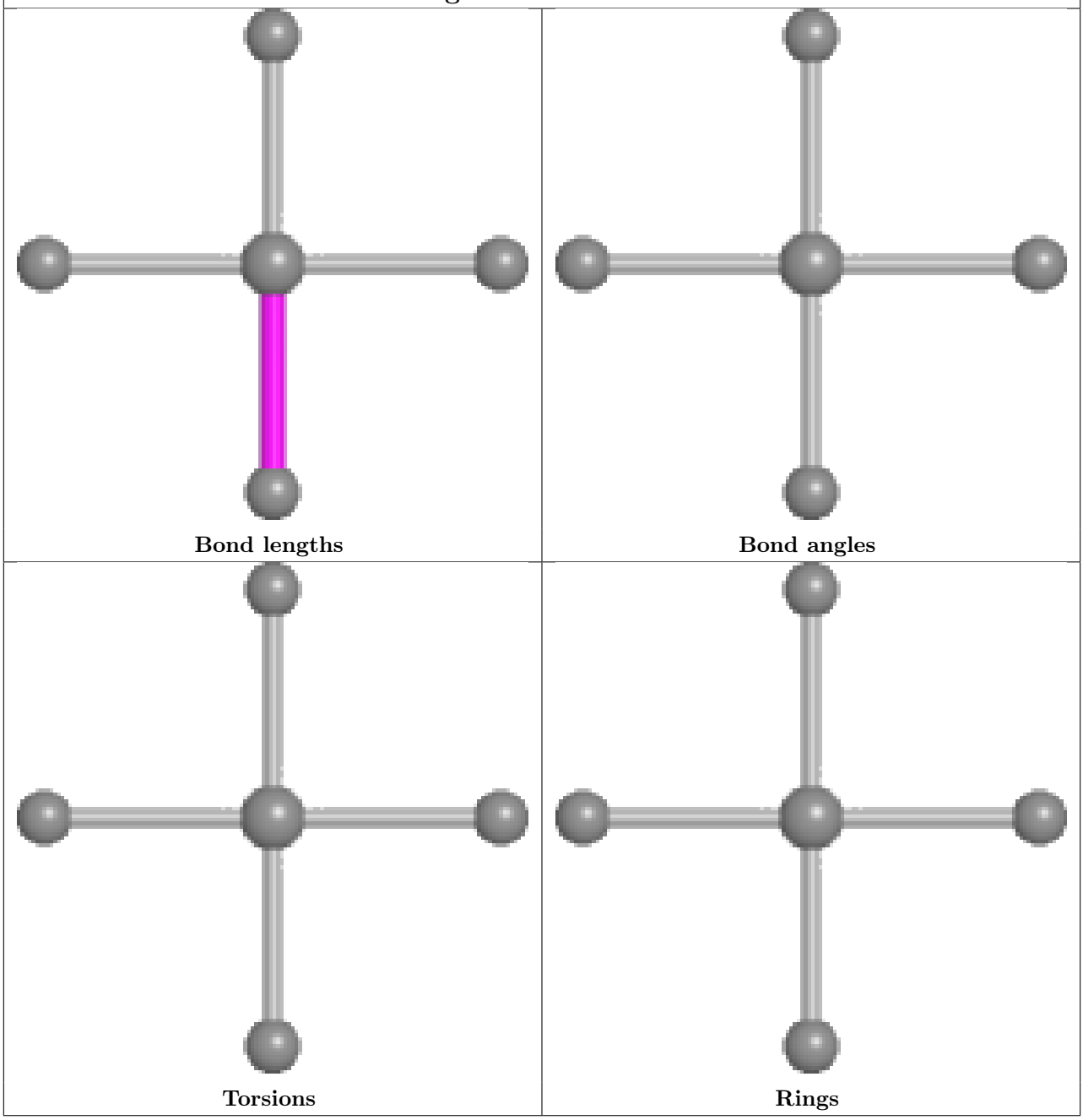


Rings

Ligand ADP B 601



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%)	1.10	96 (16%) 1 2	47, 101, 158, 202	0
1	B	576/580 (99%)	1.32	130 (22%) 0 1	40, 110, 164, 188	0
All	All	1147/1160 (98%)	1.21	226 (19%) 1 1	40, 106, 162, 202	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	LEU	11.4
1	A	59	ASN	10.6
1	B	539	ILE	8.9
1	A	58	SER	7.3
1	A	62	TYR	7.2
1	B	458	ALA	7.1
1	B	575	LEU	6.6
1	B	56	SER	6.5
1	A	60	PHE	6.4
1	B	337	LEU	6.4
1	B	63	GLU	6.4
1	B	463	VAL	6.3
1	B	457	LEU	6.0
1	B	495	PHE	6.0
1	B	5	GLN	5.9
1	B	542	LEU	5.8
1	A	274	LEU	5.7
1	B	562	PHE	5.7
1	A	65	LEU	5.6
1	A	562	PHE	5.5
1	B	60	PHE	5.3
1	B	335	PRO	5.3
1	B	464	ASN	5.1
1	B	59	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	569	ASN	4.9
1	A	324	HIS	4.9
1	B	58	SER	4.7
1	B	488	ARG	4.7
1	A	173	PHE	4.7
1	B	334	ILE	4.6
1	B	460	LEU	4.6
1	B	276	VAL	4.6
1	A	550	VAL	4.6
1	A	513	TYR	4.5
1	B	62	TYR	4.5
1	A	339	MET	4.4
1	A	559	SER	4.3
1	B	492	ALA	4.3
1	B	491	LEU	4.3
1	A	542	LEU	4.3
1	A	265	PHE	4.2
1	B	533	ILE	4.2
1	B	465	ASN	4.2
1	A	61	SER	4.1
1	B	168	PHE	4.0
1	A	558	ALA	4.0
1	A	375	SER	4.0
1	B	534	ASN	4.0
1	A	549	TYR	3.9
1	B	166	ASP	3.9
1	B	451	ILE	3.9
1	B	494	LEU	3.9
1	B	402	ILE	3.8
1	B	339	MET	3.8
1	A	571	TYR	3.8
1	B	439	LEU	3.8
1	A	376	LEU	3.7
1	A	144	SER	3.7
1	B	454	VAL	3.7
1	A	52	LEU	3.6
1	A	295	LEU	3.6
1	B	167	TRP	3.6
1	A	177	ILE	3.6
1	B	14	TYR	3.6
1	B	496	LEU	3.6
1	B	61	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	548	VAL	3.6
1	B	273	ILE	3.6
1	B	281	VAL	3.6
1	A	232	TYR	3.6
1	A	576	ALA	3.5
1	A	142	ASN	3.5
1	B	52	LEU	3.4
1	A	572	ILE	3.4
1	A	347	ILE	3.4
1	B	572	ILE	3.4
1	B	435	LEU	3.4
1	B	144	SER	3.4
1	A	49	ILE	3.3
1	B	470	LEU	3.3
1	B	177	ILE	3.3
1	A	168	PHE	3.3
1	B	566	MET	3.3
1	B	272	ASN	3.2
1	A	548	VAL	3.2
1	B	265	PHE	3.2
1	B	32	THR	3.2
1	A	63	GLU	3.2
1	A	561	HIS	3.2
1	B	502	ILE	3.2
1	B	161	VAL	3.2
1	B	277	LEU	3.2
1	B	375	SER	3.1
1	B	523	ILE	3.1
1	A	533	ILE	3.1
1	A	565	LEU	3.1
1	B	576	ALA	3.0
1	B	407	ILE	3.0
1	B	468	VAL	3.0
1	A	536	SER	3.0
1	B	173	PHE	3.0
1	B	571	TYR	3.0
1	B	493	ARG	3.0
1	A	579	THR	3.0
1	A	362	ASN	3.0
1	B	545	SER	3.0
1	A	45	ILE	2.9
1	A	39	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	99	LYS	2.9
1	B	350	LEU	2.9
1	B	503	ILE	2.9
1	B	455	LEU	2.9
1	A	161	VAL	2.9
1	B	535	ILE	2.9
1	B	146	ASN	2.9
1	A	535	ILE	2.9
1	B	536	SER	2.9
1	B	527	PHE	2.9
1	B	577	SER	2.9
1	B	293	ILE	2.8
1	A	208	LEU	2.8
1	A	9	LEU	2.8
1	B	142	ASN	2.8
1	A	338	ASN	2.8
1	A	44	LEU	2.8
1	A	503	ILE	2.8
1	A	272	ASN	2.8
1	B	286	PHE	2.8
1	A	364	VAL	2.8
1	B	307	LEU	2.7
1	B	409	LEU	2.7
1	A	14	TYR	2.7
1	B	105	TYR	2.7
1	B	547	CYS	2.7
1	B	514	ILE	2.7
1	A	242	ALA	2.7
1	B	384	LYS	2.7
1	A	346	SER	2.7
1	B	453	LYS	2.6
1	A	254	LEU	2.6
1	A	560	GLY	2.6
1	B	165	LYS	2.6
1	A	566	MET	2.6
1	A	32	THR	2.6
1	A	387	LEU	2.6
1	A	577	SER	2.6
1	B	65	LEU	2.6
1	A	534	ASN	2.6
1	A	76	VAL	2.6
1	B	140	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	515	ASN	2.6
1	B	563	ARG	2.6
1	B	296	LEU	2.6
1	A	502	ILE	2.6
1	B	158	ILE	2.6
1	A	495	PHE	2.5
1	A	246	TYR	2.5
1	B	21	GLY	2.5
1	B	289	ILE	2.5
1	B	543	GLU	2.5
1	A	404	LEU	2.5
1	A	129	LEU	2.5
1	A	79	ASN	2.5
1	B	357	ASP	2.5
1	B	574	GLY	2.5
1	B	103	LEU	2.5
1	A	286	PHE	2.5
1	B	403	TYR	2.4
1	B	476	ASN	2.4
1	B	348	ARG	2.4
1	A	539	ILE	2.4
1	B	540	ASN	2.4
1	A	243	GLN	2.4
1	A	276	VAL	2.4
1	A	67	LEU	2.4
1	A	293	ILE	2.4
1	B	486	LYS	2.4
1	B	129	LEU	2.4
1	B	377	THR	2.4
1	B	28	MET	2.3
1	A	551	LEU	2.3
1	B	6	LYS	2.3
1	B	531	LEU	2.3
1	B	551	LEU	2.3
1	A	402	ILE	2.3
1	A	106	LEU	2.3
1	B	422	TYR	2.3
1	A	245	LYS	2.2
1	B	106	LEU	2.2
1	A	64	TYR	2.2
1	A	192	ALA	2.2
1	B	86	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	538	ARG	2.2
1	B	364	VAL	2.2
1	A	460	LEU	2.2
1	B	153	GLN	2.2
1	A	567	VAL	2.2
1	B	404	LEU	2.1
1	A	313	SER	2.1
1	B	280	VAL	2.1
1	B	347	ILE	2.1
1	B	209	LEU	2.1
1	B	391	ILE	2.1
1	B	424	LEU	2.1
1	B	50	THR	2.1
1	B	431	PHE	2.1
1	B	459	ASN	2.1
1	A	281	VAL	2.1
1	A	188	THR	2.1
1	A	457	LEU	2.1
1	A	126	THR	2.1
1	A	25	PHE	2.1
1	B	561	HIS	2.1
1	B	9	LEU	2.1
1	A	312	GLN	2.1
1	B	345	LEU	2.1
1	A	219	ALA	2.0
1	A	390	ILE	2.0
1	B	376	LEU	2.0
1	B	85	LEU	2.0
1	B	481	TYR	2.0
1	A	228	ILE	2.0
1	A	361	LEU	2.0
1	A	531	LEU	2.0
1	B	57	LEU	2.0
1	B	474	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 monosaccharides in this entry.

6.4 Ligands (i)

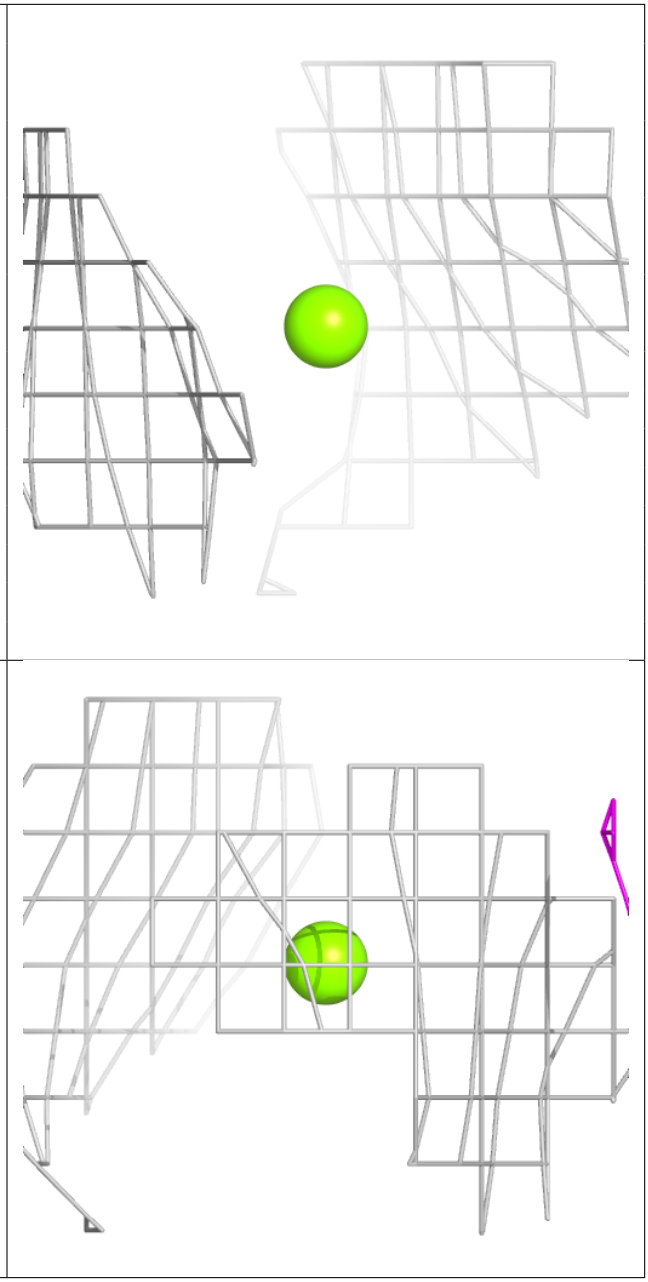
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	602	1/1	0.92	0.17	77,77,77,77	0
2	ADP	A	601	27/27	0.93	0.19	116,122,125,126	0
3	MG	B	602	1/1	0.97	0.24	37,37,37,37	0
2	ADP	B	601	27/27	0.98	0.24	60,64,68,70	0
4	VO4	A	603	5/5	0.98	0.18	103,105,106,107	0
4	VO4	B	603	5/5	0.98	0.18	87,91,91,93	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.

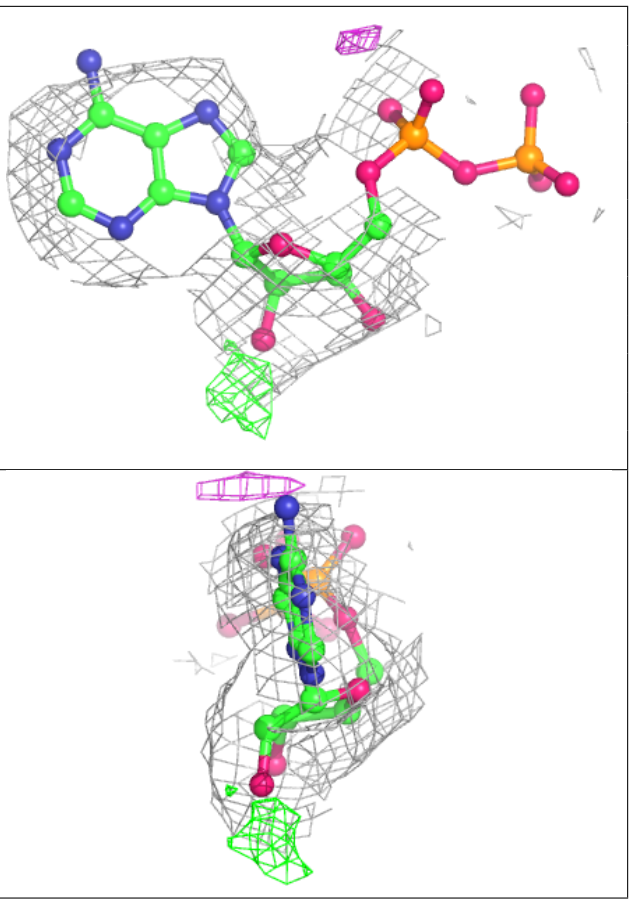
Electron density around MG A 602:

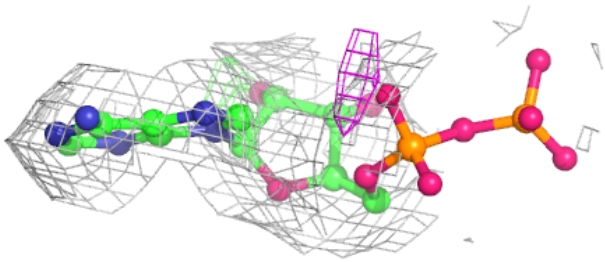
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 601:

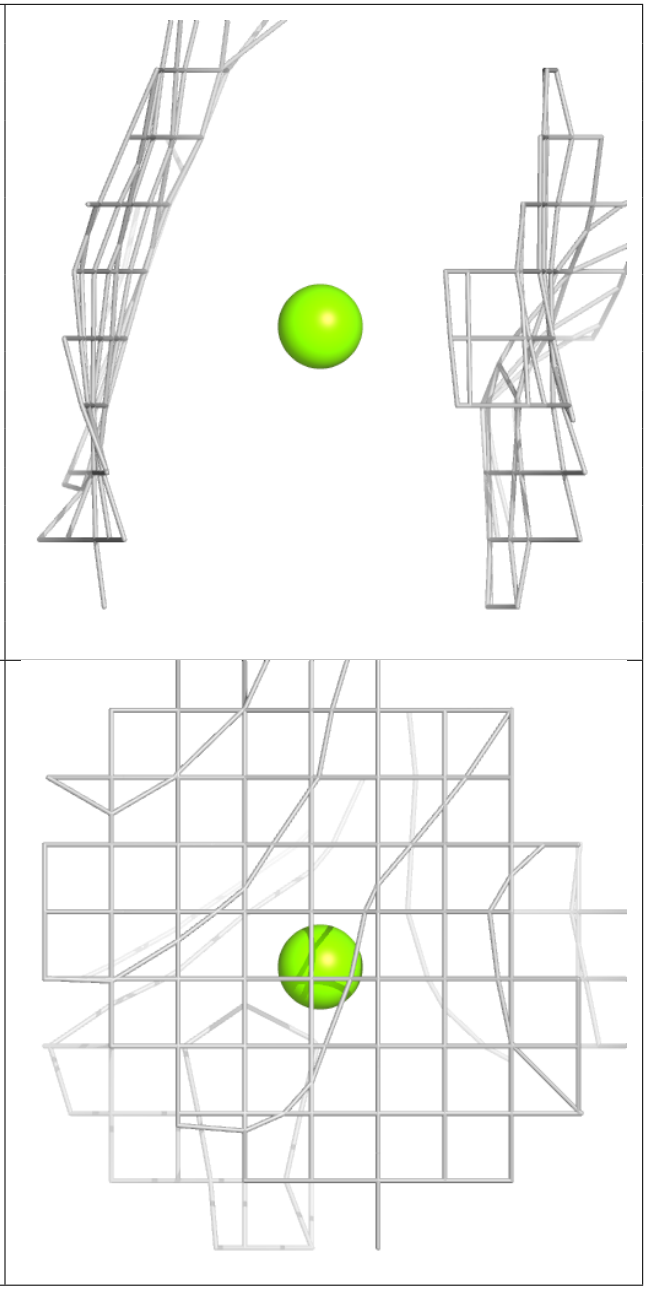
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





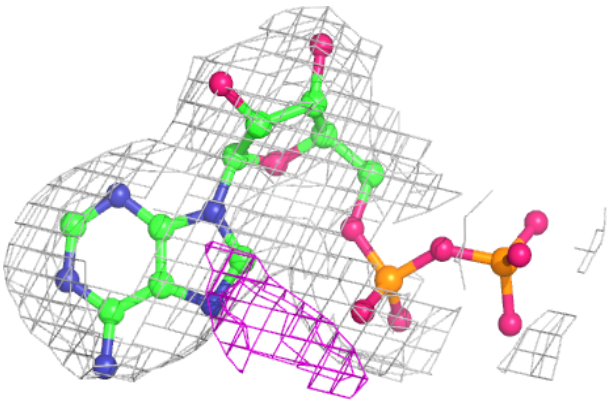
Electron density around MG B 602:

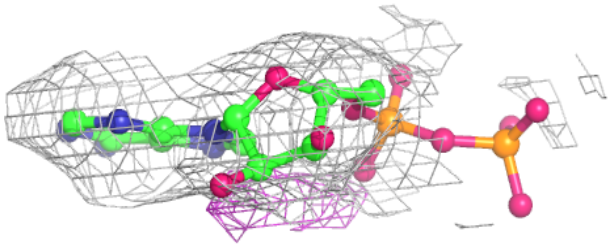
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

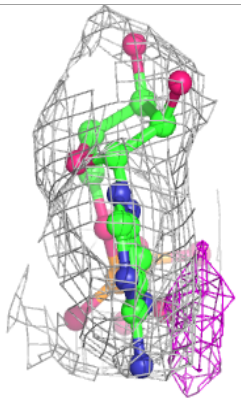


Electron density around ADP B 601:

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

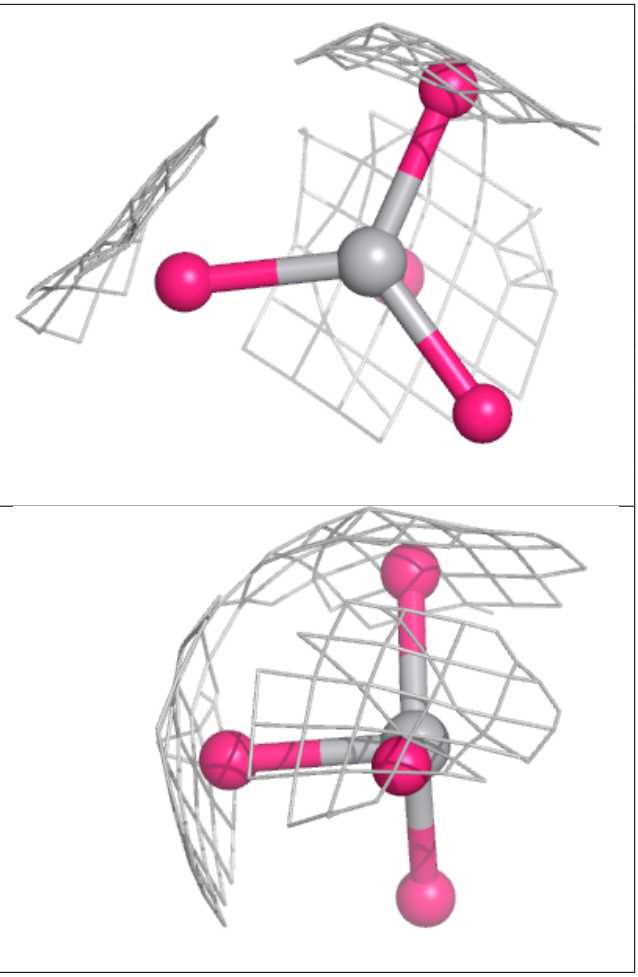






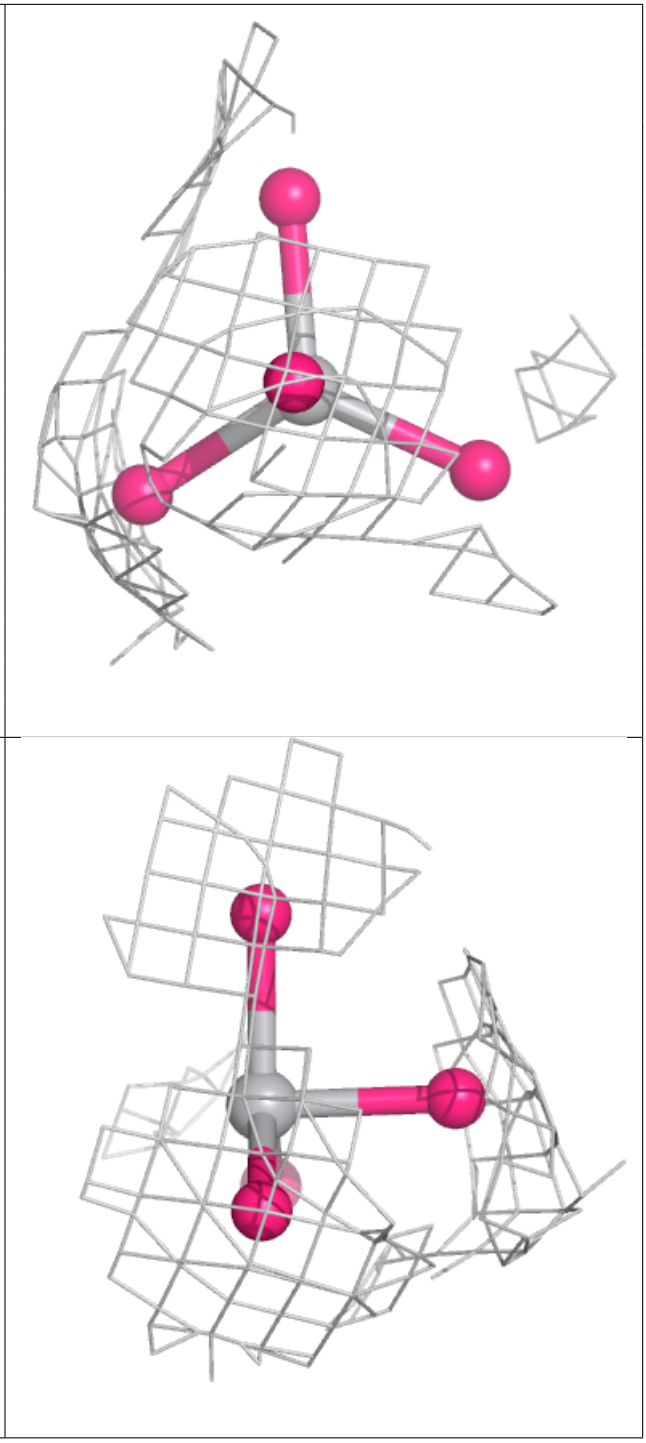
Electron density around VO4 A 603:

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)



6.5 Other polymers (i)

There are no such residues in this entry.