Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID	:	2JI9 / pdb_00002ji9
Title	:	X-ray structure of Oxalyl-CoA decarboxylase in complex with 3-deaza- ThDP
Authors	:	Berthold, C.L.; Toyota, C.G.; Moussatche, P.; Wood, M.D.; Leeper, F.; Richards, N.G.J.; Lindqvist, Y.
Deposited on	:	2007-02-26
Resolution	:	2.20 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:

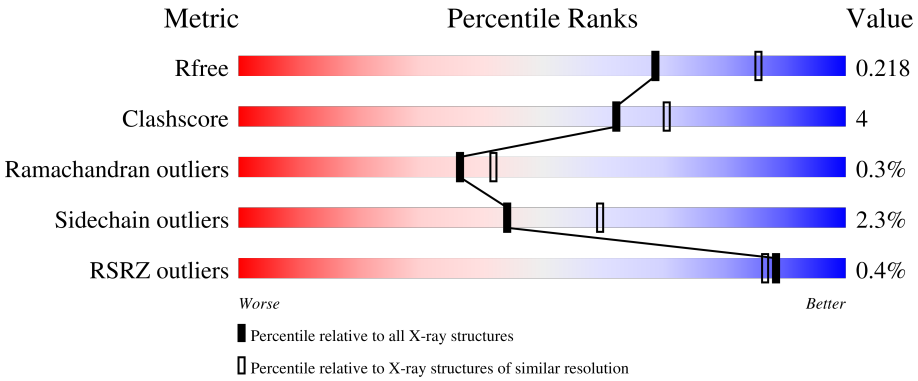
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	568	87% 9%
1	B	568	% 87% 9%

2 Entry composition (i)

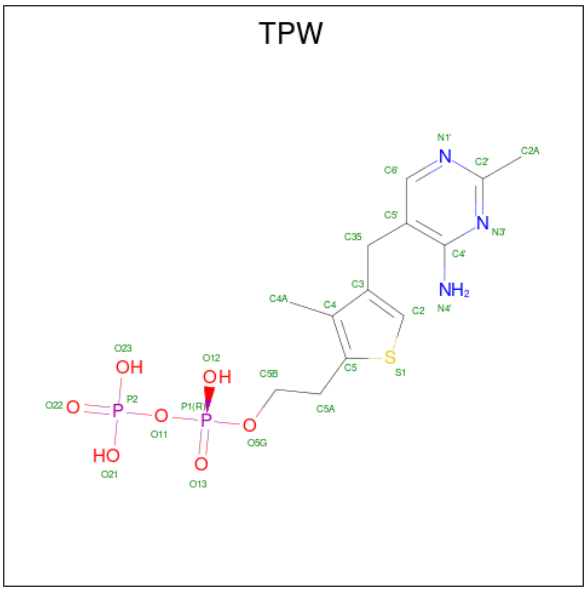
There are 6 unique types of molecules in this entry. The entry contains 8956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OXALYL-COA DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	2	0
			4094	2577	708	773	36			
1	B	547	Total	C	N	O	S	0	3	0
			4100	2581	708	775	36			

- Molecule 2 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLTHIOPHEN-2-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TPW) (formula: $C_{13}H_{19}N_3O_7P_2S$).

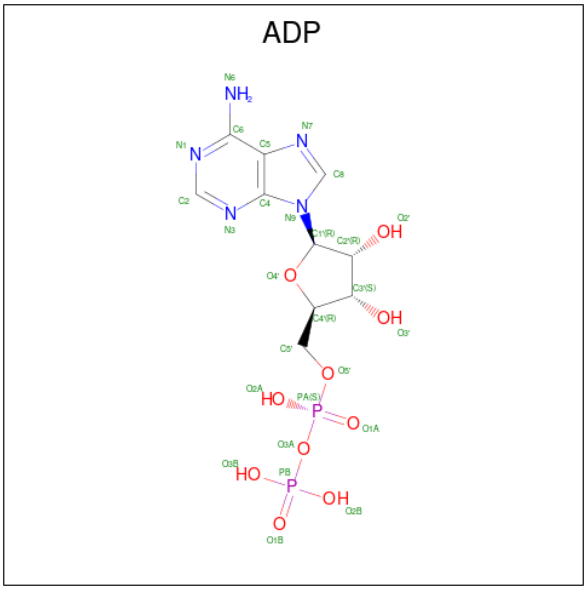


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

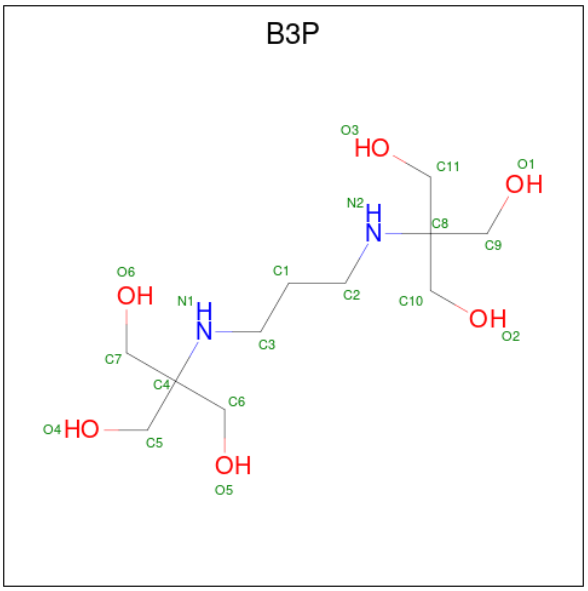
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

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



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

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 19 11 2 6	0	0
5	B	1	Total C N O 19 11 2 6	0	0

- Molecule 6 is water.

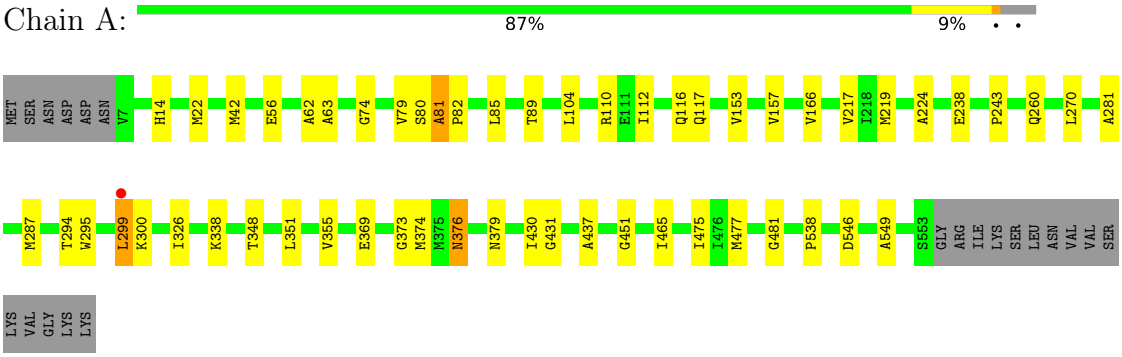
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	303	Total O 303 303	0	0
6	B	313	Total O 313 313	0	0

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.

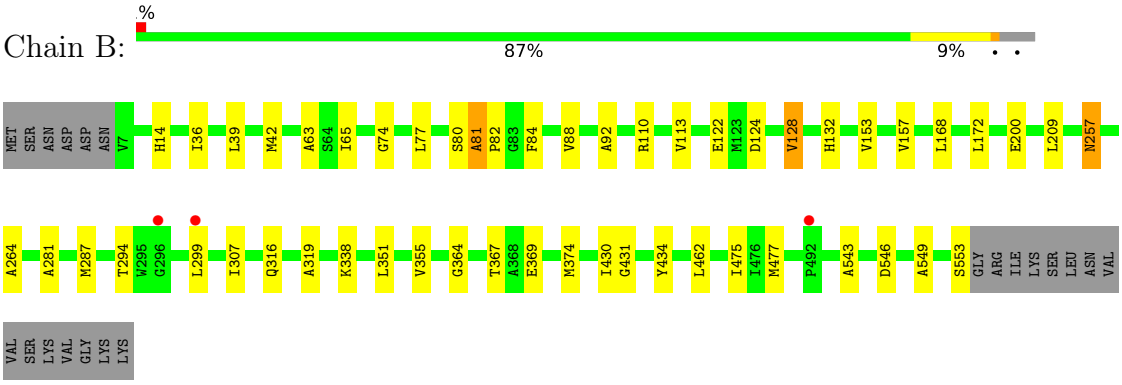
• Molecule 1: OXALYL-COA DECARBOXYLASE

Chain A:



• Molecule 1: OXALYL-COA DECARBOXYLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.72Å 127.72Å 152.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-2.20) 97.7 (30.00-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.215 0.182 , 0.218	Depositor DCC
R_{free} test set	3416 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.908	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8956	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, TPW, 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	0.59	0/4174	0.79	2/5652 (0.0%)
1	B	0.57	0/4183	0.80	1/5664 (0.0%)
All	All	0.58	0/8357	0.80	3/11316 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	36	ILE	N-CA-C	6.24	118.09	112.17
1	A	451	GLY	N-CA-C	-5.42	105.70	111.93
1	A	481	GLY	N-CA-C	5.40	118.35	110.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4094	0	4124	33	0
1	B	4100	0	4130	34	0
2	A	26	0	16	0	0
2	B	26	0	16	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	12	0	0
4	B	27	0	12	1	0
5	A	19	0	26	0	0
5	B	19	0	26	2	0
6	A	303	0	0	1	0
6	B	313	0	0	1	0
All	All	8956	0	8362	69	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 4.

All (69) 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:B:14:HIS:CE1	1:B:42:MET:HE3	2.18	0.77
1:B:14:HIS:CE1	1:B:42:MET:CE	2.70	0.74
1:A:376:ASN:HD22	1:A:376:ASN:C	1.96	0.73
1:A:373:GLY:O	1:A:374:MET:HE2	1.91	0.70
1:B:124:ASP:O	1:B:128:VAL:HG13	1.93	0.68
1:A:153:VAL:O	1:A:157:VAL:HG22	1.96	0.66
1:B:281:ALA:HB1	1:B:287:MET:HE1	1.79	0.64
1:B:81:ALA:HB3	1:B:82:PRO:CD	2.28	0.64
1:B:153:VAL:O	1:B:157:VAL:HG22	2.00	0.62
1:B:430:ILE:HD12	1:B:430:ILE:C	2.26	0.61
1:B:14:HIS:NE2	1:B:42:MET:HE3	2.16	0.60
1:B:475:ILE:HG22	1:B:477:MET:HE3	1.84	0.59
1:B:281:ALA:HB1	1:B:287:MET:CE	2.33	0.58
1:B:113:VAL:HG22	1:B:122:GLU:HG3	1.87	0.57
1:A:81:ALA:HB3	1:A:82:PRO:CD	2.35	0.57
1:A:376:ASN:HD21	1:A:379:ASN:H	1.52	0.57
1:A:351:LEU:O	1:A:355:VAL:HG23	2.05	0.56
1:B:351:LEU:O	1:B:355:VAL:HG23	2.06	0.56
1:A:219[B]:MET:SD	1:A:270:LEU:HD21	2.46	0.55
1:A:219[B]:MET:HE2	1:A:287:MET:SD	2.47	0.54
1:B:81:ALA:CB	1:B:82:PRO:CD	2.86	0.54
1:A:430:ILE:HD12	1:A:431:GLY:N	2.23	0.54
1:A:14:HIS:NE2	1:A:42:MET:HE2	2.23	0.53
1:A:546:ASP:HB3	1:A:549:ALA:HB2	1.88	0.53
1:B:200:GLU:HG2	6:B:2055:HOH:O	2.09	0.53
1:A:376:ASN:C	1:A:376:ASN:ND2	2.67	0.52
1:A:281:ALA:HB1	1:A:287:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ALA:HB3	1:B:82:PRO:HD3	1.92	0.51
1:B:14:HIS:NE2	1:B:42:MET:CE	2.73	0.51
1:A:238:GLU:HA	1:A:260:GLN:HE22	1.76	0.49
1:B:65:ILE:HD13	1:B:434:TYR:CZ	2.48	0.49
1:A:14:HIS:CE1	1:A:42:MET:CE	2.96	0.48
1:A:14:HIS:NE2	1:A:42:MET:CE	2.76	0.48
1:B:264:ALA:HB3	1:B:355:VAL:HG13	1.95	0.48
1:A:376:ASN:ND2	1:A:379:ASN:H	2.11	0.48
1:B:39:LEU:HD23	1:B:77:LEU:HD11	1.95	0.48
1:A:81:ALA:HB3	1:A:82:PRO:HD3	1.96	0.48
1:B:430:ILE:HD12	1:B:431:GLY:N	2.30	0.47
1:A:270:LEU:HD22	1:A:295:TRP:CH2	2.50	0.46
1:A:475:ILE:HG22	1:A:477:MET:HE2	1.97	0.46
1:B:307:ILE:HB	4:B:1556:ADP:C2	2.51	0.46
1:A:81:ALA:CB	1:A:82:PRO:CD	2.94	0.46
1:B:209:LEU:HD11	1:B:319:ALA:HB3	1.97	0.46
1:A:104:LEU:HD23	1:A:166:VAL:HB	1.97	0.46
1:A:224:ALA:HA	1:A:326:ILE:HD13	1.98	0.46
1:B:92:ALA:HB2	1:B:132:HIS:HB3	1.97	0.45
1:A:243:PRO:HD3	1:A:348:THR:HG22	1.99	0.45
1:A:299:LEU:HD22	1:A:300:LYS:O	2.17	0.45
1:B:63:ALA:O	1:B:74:GLY:HA3	2.17	0.45
1:A:85:LEU:O	1:A:89:THR:HG23	2.16	0.45
1:B:546:ASP:HB3	1:B:549:ALA:HB2	1.98	0.45
1:A:430:ILE:HD12	1:A:430:ILE:C	2.42	0.44
1:B:477:MET:HE2	1:B:543:ALA:HB3	2.00	0.44
1:A:63:ALA:O	1:A:74:GLY:HA3	2.18	0.43
1:B:84:PHE:HE2	1:B:128:VAL:HG22	1.83	0.43
1:B:257:ASN:C	1:B:257:ASN:HD22	2.26	0.43
1:B:364:GLY:O	1:B:367:THR:HG22	2.19	0.43
1:B:430:ILE:C	1:B:430:ILE:CD1	2.92	0.43
1:A:465:ILE:HG22	1:A:538:PRO:HB3	2.01	0.42
5:B:1557:B3P:H112	5:B:1557:B3P:H21	1.01	0.42
1:B:430:ILE:HD13	1:B:434:TYR:CD2	2.54	0.42
1:B:14:HIS:CE1	1:B:42:MET:HE1	2.54	0.42
1:B:299:LEU:HD13	1:B:316:GLN:NE2	2.35	0.41
5:B:1557:B3P:H31	5:B:1557:B3P:H51	1.75	0.41
1:A:112:ILE:HG23	1:A:117:GLN:HB2	2.01	0.41
1:B:168:LEU:HD22	1:B:172:LEU:HD23	2.02	0.41
1:A:62:ALA:HB1	1:A:437:ALA:HB2	2.03	0.41
1:A:56:GLU:OE2	2:B:1554:TPW:N1'	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLN:NE2	6:A:2057:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/568 (96%)	529 (97%)	16 (3%)	2 (0%)	30	34
1	B	548/568 (96%)	530 (97%)	17 (3%)	1 (0%)	43	51
All	All	1095/1136 (96%)	1059 (97%)	33 (3%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA
1	B	81	ALA
1	A	79	VAL

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	428/445 (96%)	419 (98%)	9 (2%)	47	63
1	B	429/445 (96%)	418 (97%)	11 (3%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	857/890 (96%)	837 (98%)	20 (2%)	44 59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	80	SER
1	A	110	ARG
1	A	217	VAL
1	A	294	THR
1	A	299	LEU
1	A	338	LYS
1	A	369	GLU
1	A	376	ASN
1	B	80	SER
1	B	88	VAL
1	B	110	ARG
1	B	128	VAL
1	B	257	ASN
1	B	294	THR
1	B	338	LYS
1	B	369	GLU
1	B	374	MET
1	B	462	LEU
1	B	553	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	48	GLN
1	A	58	HIS
1	A	117	GLN
1	A	260	GLN
1	A	288	GLN
1	A	304	GLN
1	A	308	GLN
1	A	376	ASN
1	A	391	ASN
1	B	44	GLN
1	B	183	ASN

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Mol	Chain	Res	Type
1	B	228	GLN
1	B	257	ASN
1	B	316	GLN
1	B	358	ASN
1	B	391	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	TPW	B	1554	3	25,27,27	1.44	7 (28%)	37,40,40	1.51	7 (18%)
2	TPW	A	1554	3	25,27,27	1.48	7 (28%)	37,40,40	1.55	7 (18%)
4	ADP	A	1556	-	28,29,29	1.55	6 (21%)	43,45,45	1.82	10 (23%)
5	B3P	A	1557	-	18,18,18	0.68	0	23,23,23	0.72	0
4	ADP	B	1556	-	28,29,29	1.55	6 (21%)	43,45,45	1.75	10 (23%)
5	B3P	B	1557	-	18,18,18	1.15	0	23,23,23	3.15	6 (26%)

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	TPW	B	1554	3	-	2/17/17/17	0/2/2/2
2	TPW	A	1554	3	-	3/17/17/17	0/2/2/2
4	ADP	A	1556	-	-	2/16/32/32	0/3/3/3
5	B3P	A	1557	-	-	4/28/28/28	-
4	ADP	B	1556	-	-	3/16/32/32	0/3/3/3
5	B3P	B	1557	-	-	15/28/28/28	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1556	ADP	C5-C4	5.06	1.48	1.39
4	A	1556	ADP	C5-C4	5.06	1.48	1.39
4	B	1556	ADP	PA-O3A	3.21	1.63	1.59
2	A	1554	TPW	C4'-N3'	3.17	1.39	1.35
4	A	1556	ADP	PA-O3A	3.04	1.62	1.59
2	B	1554	TPW	C3-C4	-2.97	1.36	1.45
4	A	1556	ADP	C5-C6	2.96	1.49	1.41
2	A	1554	TPW	C3-C4	-2.93	1.36	1.45
4	B	1556	ADP	C5-C6	2.75	1.48	1.41
2	B	1554	TPW	P1-O11	2.73	1.62	1.59
4	A	1556	ADP	C8-N7	2.54	1.36	1.31
4	B	1556	ADP	C8-N7	2.54	1.36	1.31
2	A	1554	TPW	C2'-N3'	2.49	1.38	1.34
2	A	1554	TPW	P1-O11	2.43	1.62	1.59
2	B	1554	TPW	C4'-N3'	2.40	1.38	1.35
2	A	1554	TPW	C2'-N1'	2.32	1.37	1.34
2	B	1554	TPW	C2'-N1'	2.25	1.37	1.34
4	B	1556	ADP	C5-N7	-2.25	1.35	1.39
2	B	1554	TPW	C2-C3	2.22	1.38	1.36
2	B	1554	TPW	C2'-N3'	2.21	1.37	1.34
2	B	1554	TPW	C6'-N1'	2.20	1.38	1.34
2	A	1554	TPW	C5'-C4'	-2.10	1.39	1.42
4	A	1556	ADP	C5-N7	-2.07	1.35	1.39
4	A	1556	ADP	C4-N9	-2.07	1.33	1.37
2	A	1554	TPW	C6'-N1'	2.06	1.38	1.34
4	B	1556	ADP	C4-N9	-2.02	1.33	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1557	B3P	C9-C8-N2	-8.14	84.73	109.02
5	B	1557	B3P	C11-C8-N2	-6.90	88.42	109.02
5	B	1557	B3P	C10-C8-N2	-6.18	90.58	109.02
5	B	1557	B3P	C11-C8-C9	6.16	123.52	110.02
4	A	1556	ADP	C5-C4-N3	-5.02	119.80	126.72
4	B	1556	ADP	C5-C4-N3	-4.81	120.09	126.72
5	B	1557	B3P	C10-C8-C9	4.15	119.12	110.02
4	A	1556	ADP	N3-C4-N9	3.97	133.92	127.17
4	B	1556	ADP	N3-C4-N9	3.95	133.89	127.17
4	B	1556	ADP	N3-C2-N1	-3.87	122.72	128.58
4	A	1556	ADP	C4-C5-N7	-3.75	106.30	110.58
4	A	1556	ADP	C2-N3-C4	3.55	120.50	111.83
4	A	1556	ADP	N3-C2-N1	-3.53	123.24	128.58
2	A	1554	TPW	C2-S1-C5	-3.52	89.08	92.41
4	B	1556	ADP	C2-N3-C4	3.52	120.43	111.83
2	A	1554	TPW	N1'-C2'-N3'	-3.42	119.84	125.53
4	B	1556	ADP	C4-C5-N7	-3.41	106.69	110.58
2	B	1554	TPW	C2-S1-C5	-3.33	89.27	92.41
2	B	1554	TPW	C6'-C5'-C4'	3.29	119.60	115.55
2	A	1554	TPW	C6'-C5'-C4'	3.22	119.51	115.55
4	A	1556	ADP	C4-N9-C8	3.21	109.11	105.74
5	B	1557	B3P	C11-C8-C10	3.15	116.93	110.02
4	B	1556	ADP	C4-N9-C8	3.13	109.03	105.74
2	B	1554	TPW	N1'-C2'-N3'	-3.07	120.43	125.53
4	A	1556	ADP	C5-N7-C8	2.79	107.84	103.45
2	A	1554	TPW	C2A-C2'-N1'	2.73	120.11	117.20
4	B	1556	ADP	C2-N1-C6	2.70	123.16	118.73
4	A	1556	ADP	C6-C5-N7	2.62	137.14	132.09
4	B	1556	ADP	C5-N7-C8	2.57	107.49	103.45
4	B	1556	ADP	C6-C5-N7	2.55	137.00	132.09
2	B	1554	TPW	C2A-C2'-N1'	2.48	119.84	117.20
2	B	1554	TPW	C5'-C6'-N1'	-2.46	119.83	123.83
4	A	1556	ADP	N9-C8-N7	-2.44	110.47	113.94
2	B	1554	TPW	C6'-N1'-C2'	2.39	119.99	116.07
2	A	1554	TPW	N4'-C4'-N3'	2.31	120.14	117.03
2	A	1554	TPW	C6'-N1'-C2'	2.30	119.85	116.07
2	B	1554	TPW	C2-C3-C4	2.28	113.53	111.92
4	B	1556	ADP	N9-C8-N7	-2.23	110.77	113.94
4	A	1556	ADP	C2-N1-C6	2.18	122.32	118.73
2	A	1554	TPW	C2'-N3'-C4'	2.06	121.26	118.10

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1557	B3P	N1-C4-C7-O6
5	B	1557	B3P	C5-C4-C7-O6
5	B	1557	B3P	C6-C4-C7-O6
5	B	1557	B3P	C10-C8-N2-C2
5	B	1557	B3P	C11-C8-N2-C2
5	B	1557	B3P	N2-C8-C9-O1
5	B	1557	B3P	C11-C8-C9-O1
5	B	1557	B3P	O2-C10-C8-N2
5	B	1557	B3P	O2-C10-C8-C11
5	B	1557	B3P	O3-C11-C8-C10
5	A	1557	B3P	C2-C1-C3-N1
4	A	1556	ADP	O4'-C4'-C5'-O5'
5	B	1557	B3P	C2-C1-C3-N1
5	A	1557	B3P	C1-C2-N2-C8
5	B	1557	B3P	C1-C2-N2-C8
4	A	1556	ADP	C3'-C4'-C5'-O5'
5	A	1557	B3P	C3-C1-C2-N2
4	B	1556	ADP	O4'-C4'-C5'-O5'
5	B	1557	B3P	C1-C3-N1-C4
4	B	1556	ADP	C3'-C4'-C5'-O5'
5	B	1557	B3P	C9-C8-N2-C2
2	A	1554	TPW	P1-O11-P2-O22
5	A	1557	B3P	C1-C3-N1-C4
5	B	1557	B3P	C5-C4-N1-C3
2	A	1554	TPW	P1-O11-P2-O21
2	A	1554	TPW	P1-O11-P2-O23
2	B	1554	TPW	P1-O11-P2-O21
2	B	1554	TPW	P1-O11-P2-O23
4	B	1556	ADP	PB-O3A-PA-O2A

There are no ring outliers.

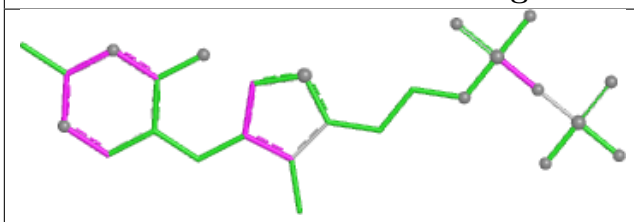
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1554	TPW	1	0
4	B	1556	ADP	1	0
5	B	1557	B3P	2	0

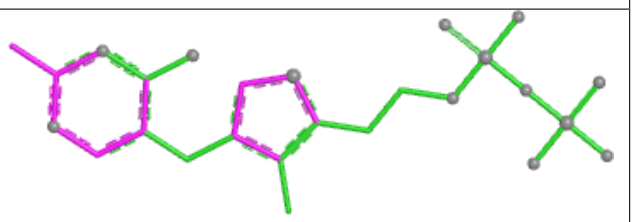
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

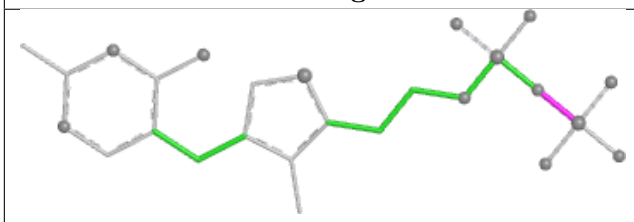
Ligand TPW B 1554



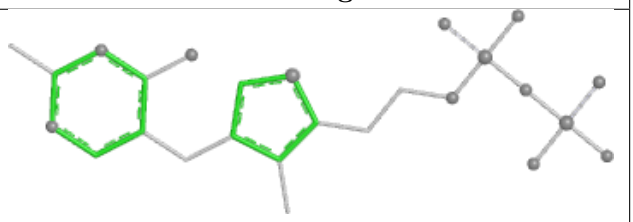
Bond lengths



Bond angles

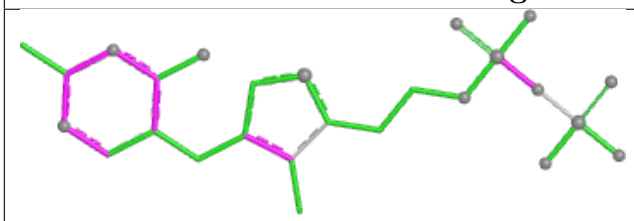


Torsions

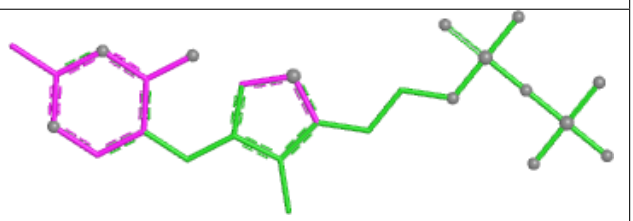


Rings

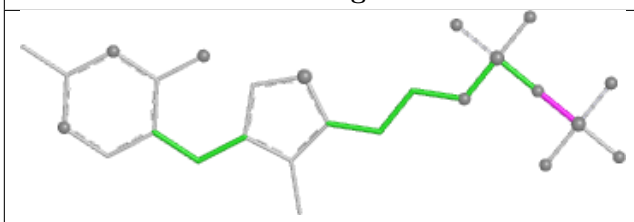
Ligand TPW A 1554



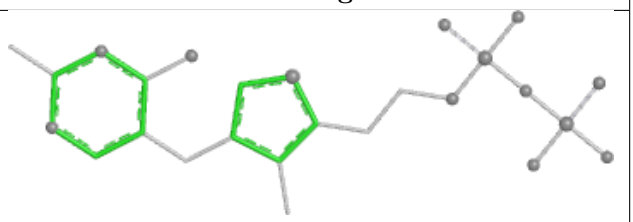
Bond lengths



Bond angles

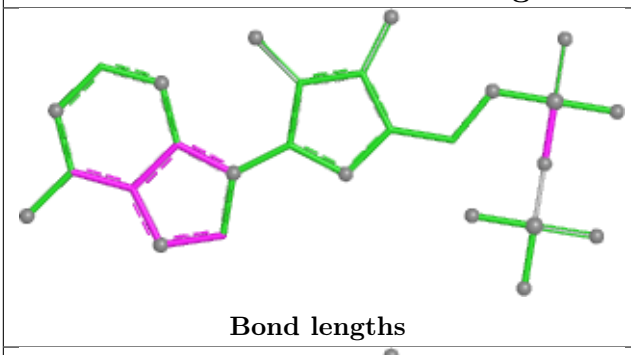


Torsions

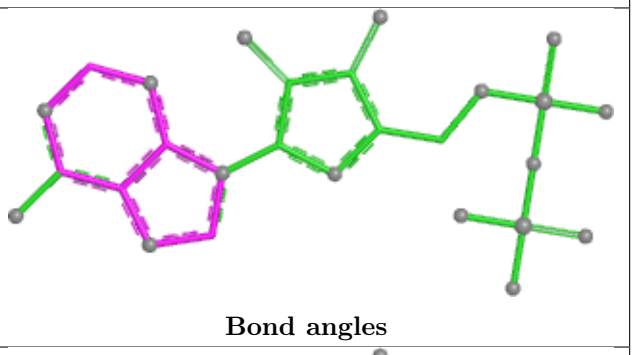


Rings

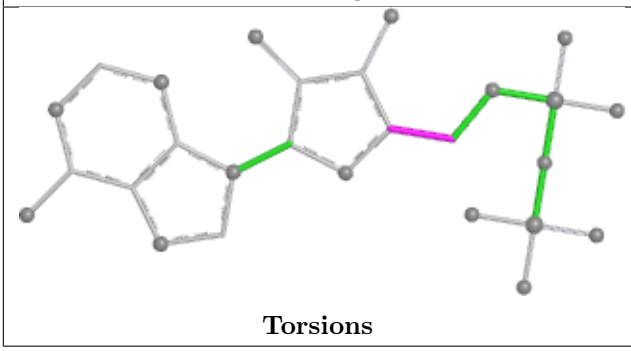
Ligand ADP A 1556



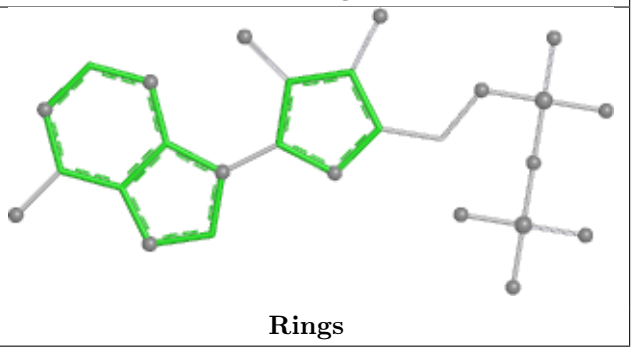
Bond lengths



Bond angles

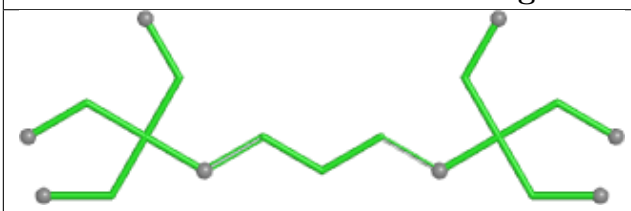


Torsions

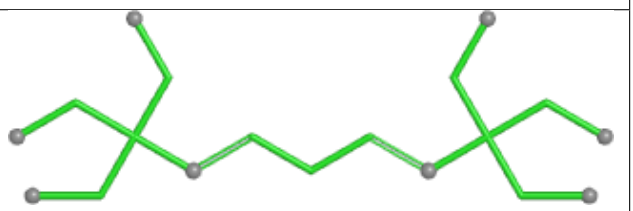


Rings

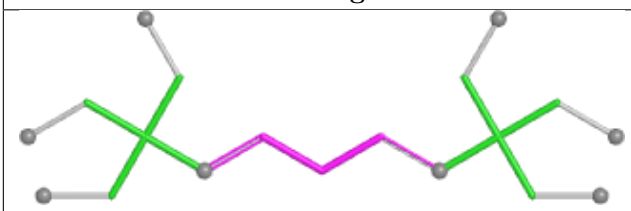
Ligand B3P A 1557



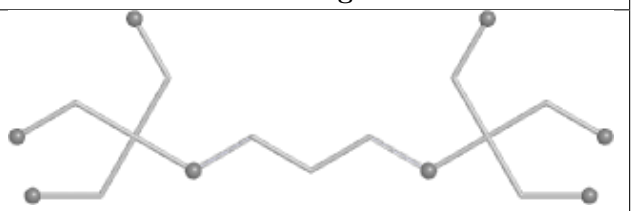
Bond lengths



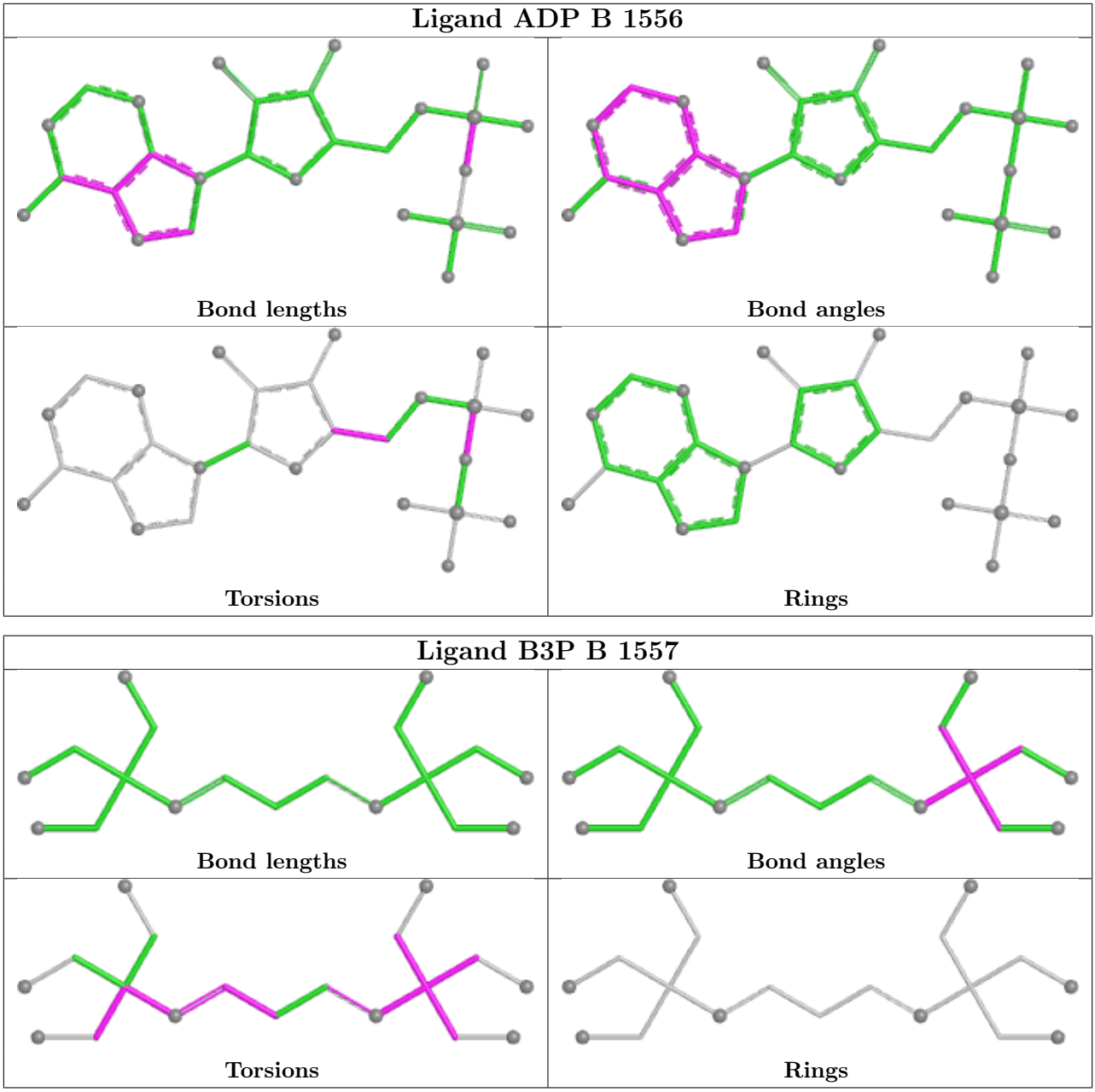
Bond angles



Torsions



Rings



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	547/568 (96%)	-0.10	1 (0%)	91	90	23, 38, 48, 60	2 (0%)
1	B	547/568 (96%)	-0.09	3 (0%)	87	85	24, 39, 48, 59	3 (0%)
All	All	1094/1136 (96%)	-0.09	4 (0%)	88	87	23, 39, 48, 60	5 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	492	PRO	2.6
1	B	299	LEU	2.5
1	B	296	GLY	2.1
1	A	299	LEU	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	B3P	A	1557	19/19	0.69	0.16	71,78,85,86	0

Continued on next page...

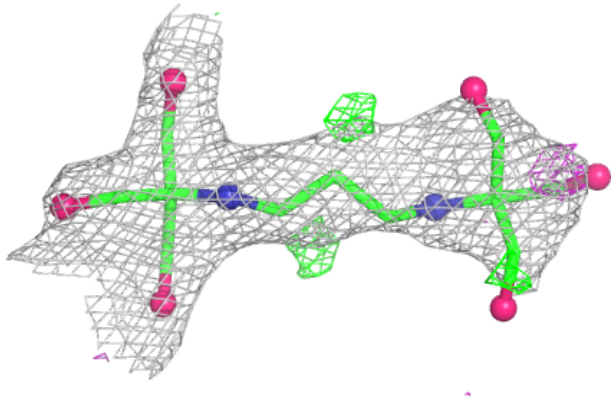
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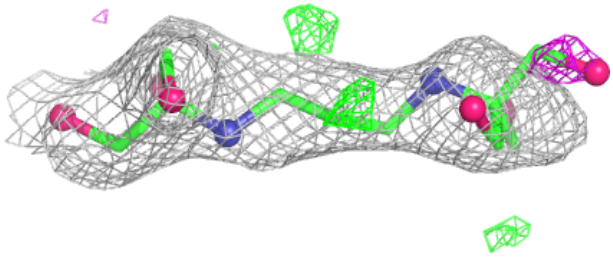
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	B3P	B	1557	19/19	0.74	0.14	70,76,83,83	0
4	ADP	A	1556	27/27	0.93	0.10	42,45,46,46	0
4	ADP	B	1556	27/27	0.93	0.11	41,44,45,45	0
2	TPW	A	1554	26/26	0.97	0.07	26,29,33,34	0
2	TPW	B	1554	26/26	0.97	0.08	30,33,34,36	0
3	MG	A	1555	1/1	0.98	0.06	26,26,26,26	0
3	MG	B	1555	1/1	0.99	0.06	36,36,36,36	0

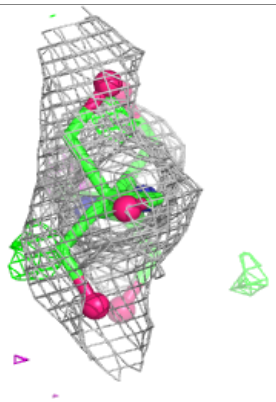
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P A 1557:

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

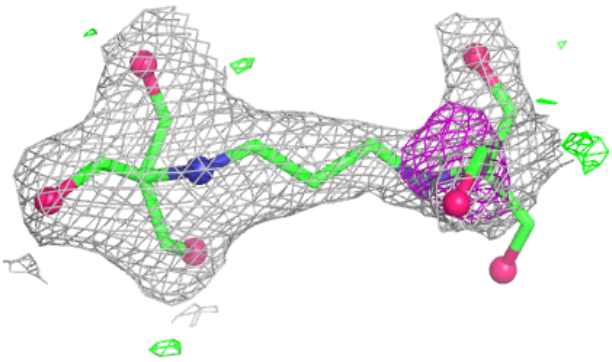


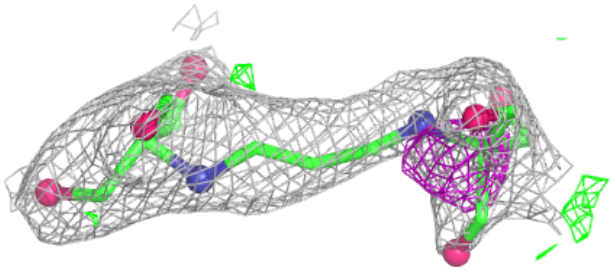


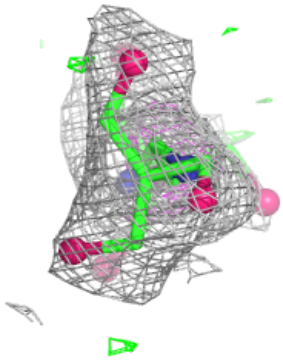


Electron density around B3P B 1557:

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

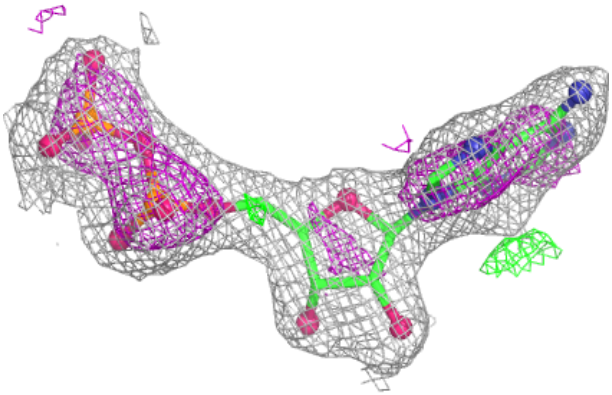


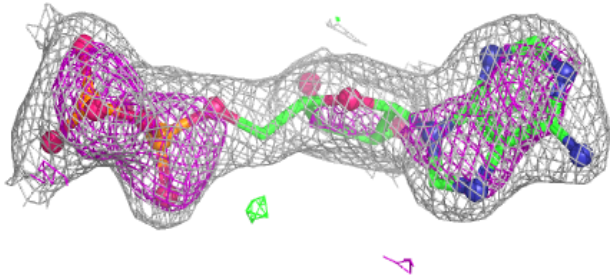


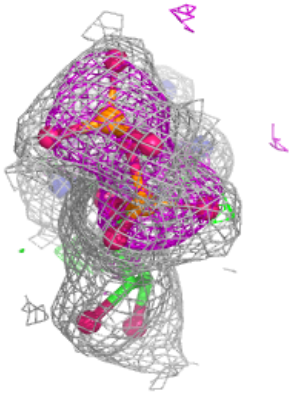


Electron density around ADP A 1556:

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

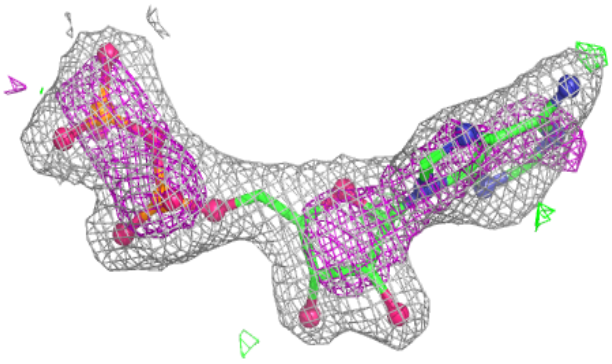


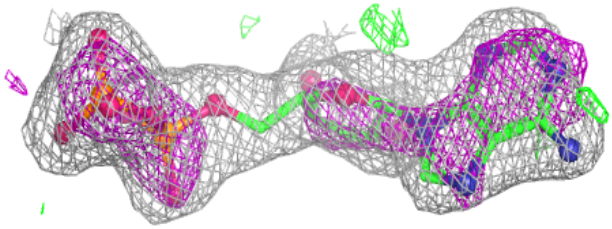


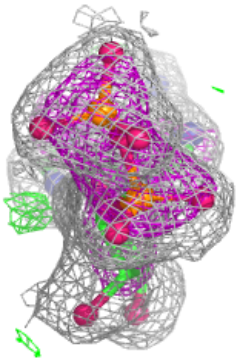


Electron density around ADP B 1556:

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

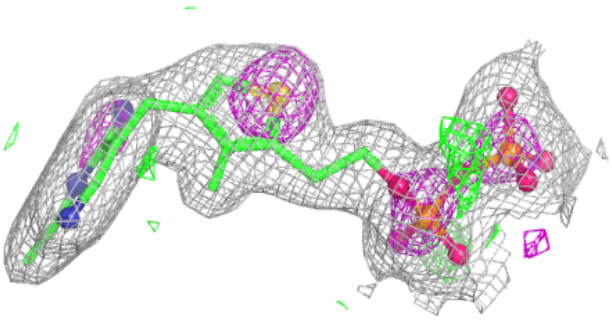


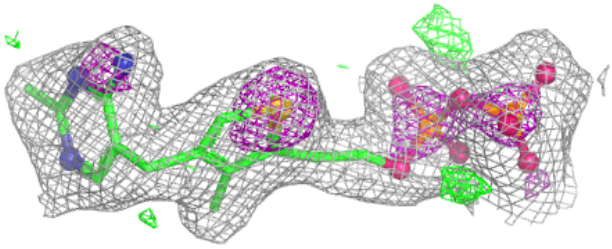


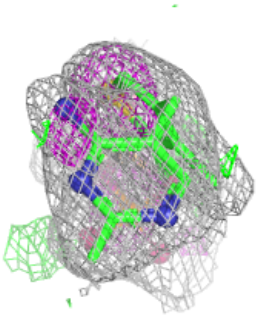


Electron density around TPW A 1554:

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

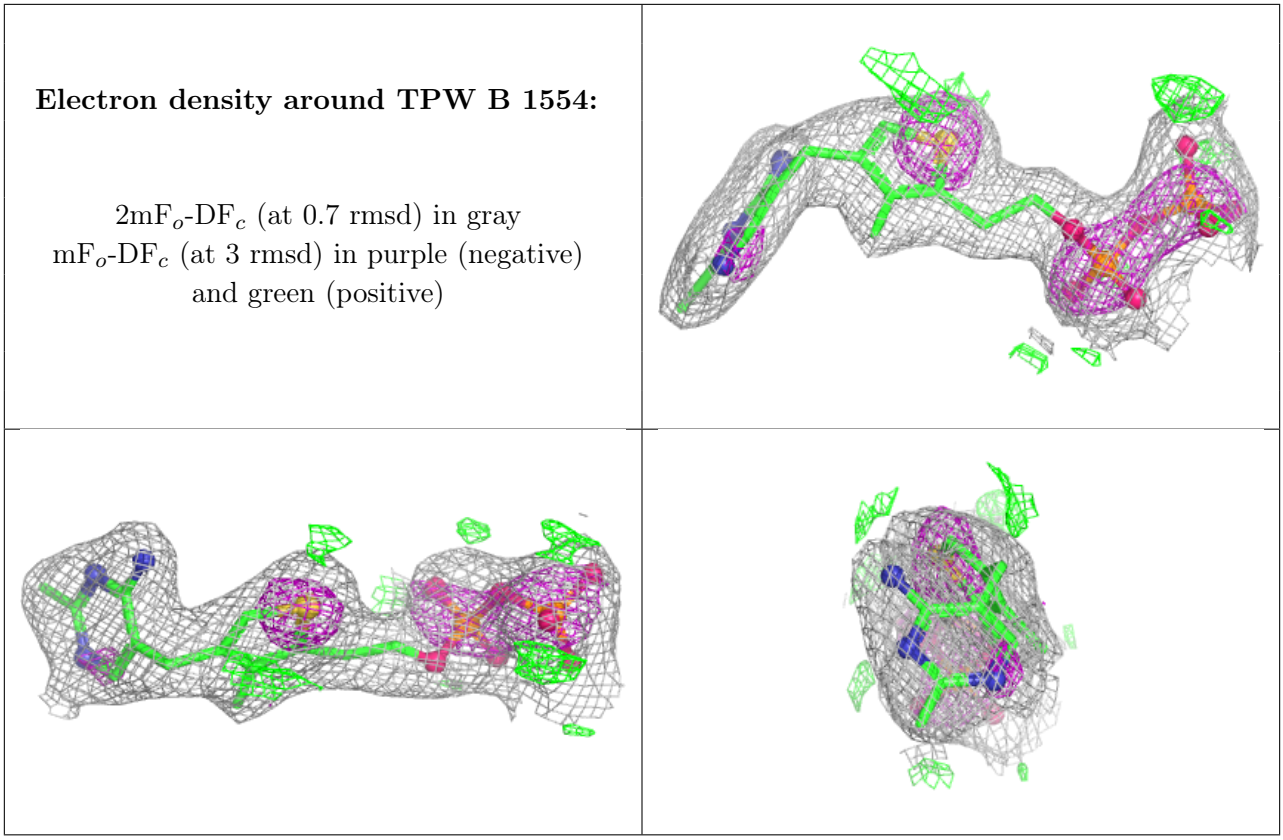






Electron density around TPW B 1554:

$2mF_o$-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.