



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:47 am BST

PDB ID : 2JI7
Title : X-ray structure of Oxalyl-CoA decarboxylase with covalent reaction intermediate
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 : 1.82 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

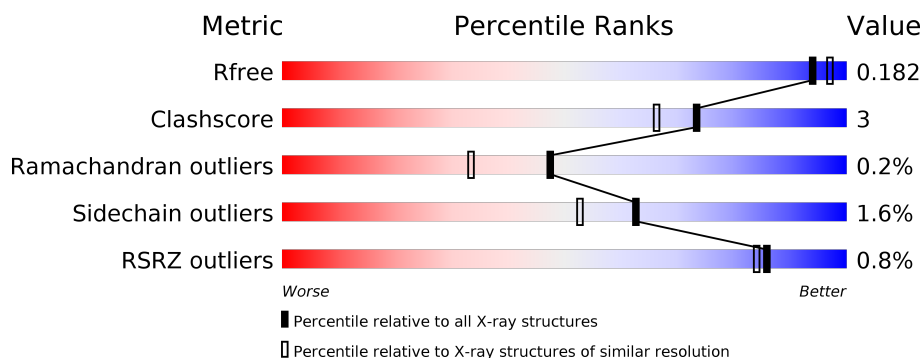
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	568	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>5% ..</div> </div> </div>
1	B	568	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6% .</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	B3P	B	1570	-	-	-	X

2 Entry composition [i](#)

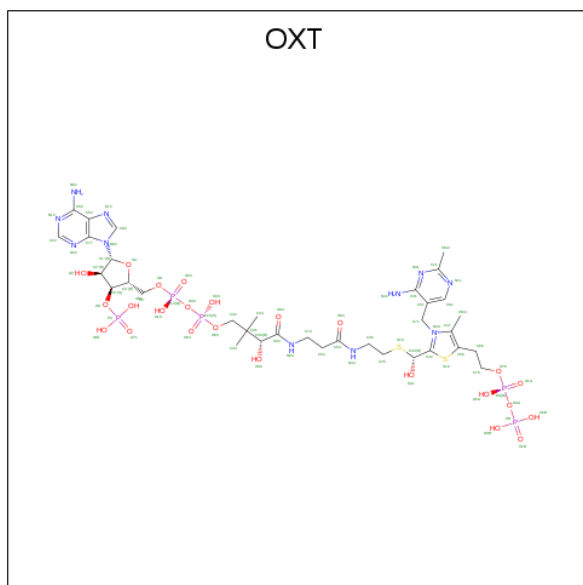
There are 7 unique types of molecules in this entry. The entry contains 9966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	559	Total	C	N	O	S	0	9	0
			4220	2663	727	791	39			
1	B	559	Total	C	N	O	S	0	9	0
			4219	2660	728	792	39			

- Molecule 2 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-{(1R,11R,15S,17R)-19-[(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOOXY)TETRAHYDROFURAN-2-YL]-1,11,15,17-TETRAHYDROXY-12,12-DIMETHYL-15,17-DIOXIDO-6,10-DIOXO-14,16,18-TRIOXA-2-THIA-5,9-DIAZA-15,17-DIPHOSPHANONAD EC-1-YL}-5-(2-{[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: OXT) (formula: C₃₄H₅₅N₁₁O₂₄P₅S₂).

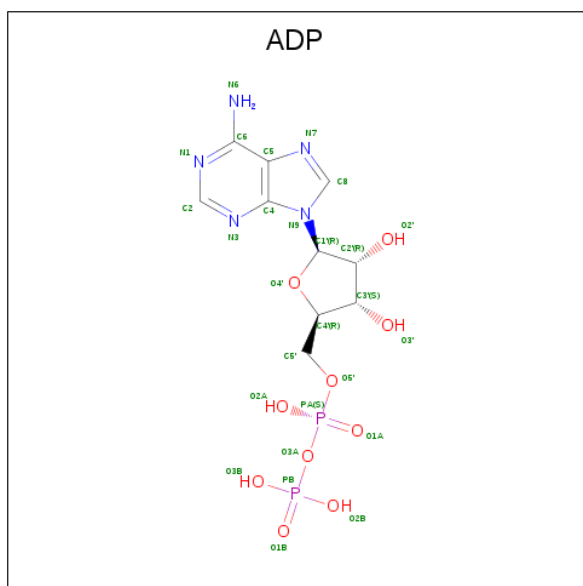


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			76	34	11	24	5 2		
2	B	1	Total	C	N	O	P S	0	0
			76	34	11	24	5 2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



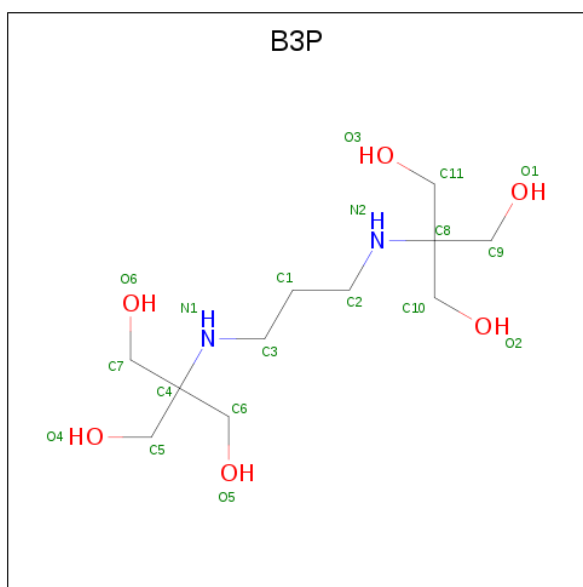
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



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

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

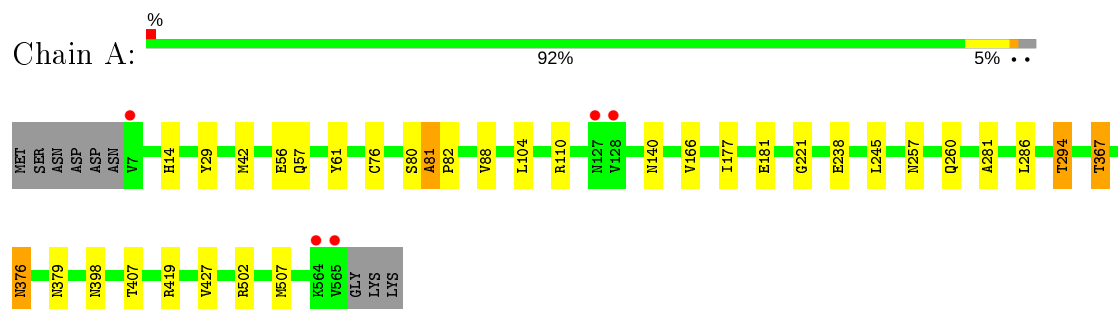
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	593	Total	O	0	0
			593	593		
7	B	592	Total	O	0	0
			592	592		

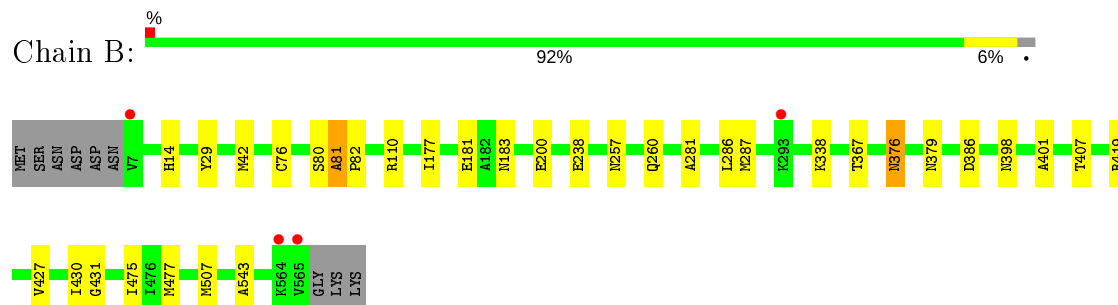
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: OXALYL-COA DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.18Å 126.18Å 151.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.82 62.38 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-1.82) 99.1 (62.38-1.82)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.150 , 0.176 0.158 , 0.182	Depositor DCC
R_{free} test set	5834 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9966	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXT, MG, PGE, B3P, ADP

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	0.37	0/4321	0.56	2/5847 (0.0%)
1	B	0.36	0/4320	0.54	0/5846
All	All	0.36	0/8641	0.55	2/11693 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	367	THR	OG1-CB-CG2	5.18	121.91	110.00
1	A	367	THR	CA-CB-CG2	5.02	119.43	112.40

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	4220	0	4292	28	0
1	B	4219	0	4285	34	0
2	A	76	0	48	2	0
2	B	76	0	48	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	0	0
5	A	10	0	14	0	0
5	B	10	0	14	0	0
6	A	57	0	78	1	0
6	B	57	0	78	3	0
7	A	593	0	0	4	1
7	B	592	0	0	4	0
All	All	9966	0	8881	59	1

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 3.

All (59) 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)
7:A:2032:HOH:O	2:B:1566:OXT:H40	1.68	0.91
2:A:1566:OXT:H40	7:B:2039:HOH:O	1.72	0.87
1:B:475:ILE:HG22	1:B:477:MET:HE3	1.59	0.84
1:A:507[B]:MET:HG2	1:B:507[B]:MET:HG2	1.57	0.84
1:A:294:THR:HG23	7:A:2323:HOH:O	1.78	0.82
1:B:477:MET:HE2	1:B:543:ALA:HB3	1.72	0.71
2:B:1566:OXT:S15	7:B:2559:HOH:O	2.48	0.71
1:B:386:ASP:OD2	6:B:1570:B3P:H22	1.93	0.68
1:B:475:ILE:HG22	1:B:477:MET:CE	2.25	0.67
6:A:1571:B3P:H62	7:A:2398:HOH:O	2.01	0.60
1:A:507[B]:MET:HG3	1:B:507[B]:MET:CE	2.33	0.59
1:B:367:THR:HG22	6:B:1570:B3P:H111	1.85	0.59
1:B:238:GLU:HA	1:B:260:GLN:HE22	1.68	0.58
1:B:81:ALA:HB3	1:B:82:PRO:CD	2.36	0.55
1:B:14:HIS:CE1	1:B:42:MET:CE	2.90	0.54
1:A:238:GLU:HA	1:A:260:GLN:HE22	1.72	0.54
1:A:398:ASN:HD22	1:A:419:ARG:HH22	1.58	0.51
1:B:430:ILE:HD12	1:B:431:GLY:N	2.26	0.50
1:A:507[B]:MET:HG3	1:B:507[B]:MET:HE3	1.93	0.50
1:B:14:HIS:CE1	1:B:42:MET:HE1	2.47	0.50
1:B:398:ASN:HD22	1:B:419:ARG:HH22	1.59	0.50
1:B:367:THR:CG2	6:B:1570:B3P:H111	2.42	0.49
1:A:398:ASN:HD21	1:A:407:THR:HB	1.77	0.48
1:A:82:PRO:HB3	1:B:427:VAL:HG22	1.97	0.47
1:A:14:HIS:NE2	1:A:42:MET:HE3	2.30	0.47
1:A:376:ASN:C	1:A:376:ASN:HD22	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ALA:HB3	1:B:82:PRO:HD3	1.97	0.47
1:B:14:HIS:CE1	1:B:42:MET:HE3	2.51	0.46
1:B:200:GLU:HG2	7:B:2108:HOH:O	2.15	0.46
1:A:81:ALA:HB3	1:A:82:PRO:CD	2.46	0.46
1:A:29:TYR:O	1:A:76:CYS:HA	2.16	0.46
1:B:29:TYR:O	1:B:76:CYS:HA	2.16	0.46
1:A:507[B]:MET:CG	1:B:507[B]:MET:HG2	2.38	0.45
1:A:140:ASN:ND2	7:A:2166:HOH:O	2.50	0.45
1:B:183[B]:ASN:ND2	7:B:2218:HOH:O	2.49	0.45
1:A:376:ASN:ND2	1:A:379:ASN:H	2.15	0.45
1:A:14:HIS:CE1	1:A:42:MET:CE	3.00	0.44
1:B:81:ALA:CB	1:B:82:PRO:CD	2.96	0.44
1:A:56:GLU:OE2	2:B:1566:OXT:N11	2.51	0.44
1:A:221:GLY:HA3	1:A:281:ALA:HB2	2.01	0.43
1:A:14:HIS:CE1	1:A:42:MET:HE3	2.54	0.43
1:A:286:LEU:O	2:A:1566:OXT:H333	2.19	0.43
1:A:507[B]:MET:HG2	1:B:507[B]:MET:CG	2.40	0.43
1:B:376:ASN:ND2	1:B:379:ASN:H	2.17	0.43
1:A:398:ASN:ND2	1:A:407:THR:HB	2.34	0.42
1:B:398:ASN:HD21	1:B:407:THR:HB	1.84	0.42
1:A:398:ASN:HD22	1:A:419:ARG:HH12	1.66	0.42
1:B:475:ILE:CG2	1:B:477:MET:CE	2.95	0.42
1:B:401:ALA:HB3	2:B:1566:OXT:O1B	2.20	0.42
1:B:286:LEU:O	2:B:1566:OXT:H333	2.20	0.42
1:A:81:ALA:HB3	1:A:82:PRO:HD3	2.00	0.42
1:A:427:VAL:HG22	1:B:82:PRO:HB3	2.01	0.41
1:B:177:ILE:HD11	1:B:181:GLU:HG2	2.01	0.41
1:B:281:ALA:HB1	1:B:287[A]:MET:CE	2.50	0.41
1:A:57:GLN:HG2	1:A:61:TYR:CE2	2.56	0.41
1:B:430:ILE:HD12	1:B:430:ILE:C	2.41	0.41
1:B:376:ASN:HD22	1:B:376:ASN:C	2.23	0.41
1:A:104:LEU:HD23	1:A:166:VAL:HB	2.03	0.41
1:A:177:ILE:HD11	1:A:181:GLU:HG2	2.02	0.40

All (1) 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)
7:A:2245:HOH:O	7:A:2541:HOH:O[3_654]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/568 (100%)	552 (98%)	13 (2%)	1 (0%)	47	33
1	B	566/568 (100%)	550 (97%)	15 (3%)	1 (0%)	47	33
All	All	1132/1136 (100%)	1102 (97%)	28 (2%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/445 (100%)	437 (98%)	9 (2%)	55	43
1	B	446/445 (100%)	441 (99%)	5 (1%)	73	67
All	All	892/890 (100%)	878 (98%)	14 (2%)	62	53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	88	VAL
1	A	110	ARG
1	A	245	LEU

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Mol	Chain	Res	Type
1	A	257	ASN
1	A	294	THR
1	A	367	THR
1	A	376	ASN
1	A	502	ARG
1	B	80	SER
1	B	110	ARG
1	B	257	ASN
1	B	338	LYS
1	B	376	ASN

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

Mol	Chain	Res	Type
1	A	48	GLN
1	A	140	ASN
1	A	183	ASN
1	A	228	GLN
1	A	257	ASN
1	A	260	GLN
1	A	376	ASN
1	A	398	ASN
1	B	48	GLN
1	B	116	GLN
1	B	140	ASN
1	B	228	GLN
1	B	257	ASN
1	B	260	GLN
1	B	376	ASN
1	B	398	ASN
1	B	520	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z > 2$
5	PGE	B	1569	-	9,9,9	0.46	0	8,8,8	0.30	0
6	B3P	A	1571	-	18,18,18	0.89	1 (5%)	21,23,23	3.80	7 (33%)
4	ADP	A	1568	-	24,29,29	1.05	1 (4%)	29,45,45	1.39	5 (17%)
2	OXT	A	1566	3	64,80,80	0.97	2 (3%)	81,121,121	1.58	14 (17%)
6	B3P	B	1571	-	18,18,18	1.55	2 (11%)	21,23,23	4.08	7 (33%)
5	PGE	A	1569	-	9,9,9	0.45	0	8,8,8	0.24	0
6	B3P	B	1570	-	18,18,18	1.49	2 (11%)	21,23,23	3.91	6 (28%)
6	B3P	A	1570	-	18,18,18	0.66	0	21,23,23	0.73	1 (4%)
4	ADP	B	1568	-	24,29,29	1.02	1 (4%)	29,45,45	1.33	4 (13%)
6	B3P	B	1572	-	18,18,18	0.83	0	21,23,23	0.86	2 (9%)
2	OXT	B	1566	3	64,80,80	1.00	2 (3%)	81,121,121	1.60	16 (19%)
6	B3P	A	1572	-	18,18,18	0.75	0	21,23,23	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	B	1569	-	-	5/7/7/7	-
6	B3P	A	1571	-	-	6/28/28/28	-
4	ADP	A	1568	-	-	2/12/32/32	0/3/3/3
2	OXT	A	1566	3	-	7/61/88/88	0/5/5/5
6	B3P	B	1571	-	-	8/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	A	1569	-	-	2/7/7/7	-
6	B3P	B	1570	-	-	11/28/28/28	-
6	B3P	A	1570	-	-	3/28/28/28	-
4	ADP	B	1568	-	-	2/12/32/32	0/3/3/3
6	B3P	B	1572	-	-	7/28/28/28	-
2	OXT	B	1566	3	-	7/61/88/88	0/5/5/5
6	B3P	A	1572	-	-	10/28/28/28	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1571	B3P	C6-C4	5.51	1.60	1.53
2	B	1566	OXT	C25-S15	-5.16	1.74	1.81
2	A	1566	OXT	C25-S15	-5.15	1.74	1.81
6	B	1570	B3P	C6-C4	4.79	1.59	1.53
6	B	1570	B3P	C7-C4	3.06	1.57	1.53
6	A	1571	B3P	C7-C4	2.78	1.56	1.53
6	B	1571	B3P	C7-C4	2.75	1.56	1.53
4	B	1568	ADP	C5-C4	2.58	1.47	1.40
4	A	1568	ADP	C5-C4	2.42	1.47	1.40
2	B	1566	OXT	C66-C56	2.23	1.51	1.50
2	A	1566	OXT	C51-C41	-2.09	1.39	1.42

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1571	B3P	C7-C4-C5	-10.79	87.23	110.04
6	A	1571	B3P	C7-C4-C5	-10.69	87.43	110.04
6	B	1571	B3P	C7-C4-C6	-10.61	87.61	110.04
6	B	1570	B3P	C7-C4-C6	-10.52	87.79	110.04
6	B	1570	B3P	C7-C4-C5	-10.22	88.43	110.04
6	A	1571	B3P	C7-C4-C6	-9.42	90.12	110.04
6	B	1570	B3P	C7-C4-N1	-6.91	88.24	109.03
6	A	1571	B3P	C7-C4-N1	-6.57	89.26	109.03
6	B	1571	B3P	C7-C4-N1	-6.54	89.36	109.03
2	B	1566	OXT	C66-C56-C47	5.45	131.81	127.43
2	A	1566	OXT	N32-C22-N12	-5.11	120.69	128.68
6	B	1571	B3P	C6-C4-C5	5.10	120.83	110.04
2	B	1566	OXT	N32-C22-N12	-5.06	120.77	128.68
2	A	1566	OXT	C66-C56-C47	4.84	131.32	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1571	B3P	C3-N1-C4	-4.43	109.80	116.08
6	B	1570	B3P	C6-C4-N1	4.35	122.11	109.03
6	A	1571	B3P	C6-C4-N1	3.95	120.92	109.03
6	A	1571	B3P	C5-C4-N1	3.94	120.89	109.03
6	A	1571	B3P	C6-C4-C5	3.80	118.08	110.04
6	B	1570	B3P	C6-C4-C5	3.79	118.06	110.04
4	A	1568	ADP	N3-C2-N1	-3.68	122.93	128.68
6	B	1570	B3P	C5-C4-N1	3.49	119.52	109.03
6	B	1571	B3P	C5-C4-N1	3.47	119.46	109.03
4	B	1568	ADP	N3-C2-N1	-3.45	123.29	128.68
6	B	1571	B3P	C6-C4-N1	3.44	119.36	109.03
2	B	1566	OXT	C64-C74-N84	-3.38	105.08	111.90
2	B	1566	OXT	C25-C35-N44	-3.29	105.50	112.42
2	A	1566	OXT	C61-N11-C21	3.20	121.41	115.96
2	A	1566	OXT	N11-C21-N31	-3.17	120.08	125.54
2	A	1566	OXT	C25-C35-N44	-3.07	105.97	112.42
2	B	1566	OXT	CM4-C47-C56	-3.04	120.94	127.60
2	B	1566	OXT	C61-N11-C21	3.03	121.12	115.96
2	B	1566	OXT	CM4-C47-N43	3.02	126.49	122.69
2	A	1566	OXT	CM4-C47-N43	2.97	126.43	122.69
2	A	1566	OXT	C64-C74-N84	-2.96	105.92	111.90
4	B	1568	ADP	C4-C5-N7	-2.94	106.33	109.40
2	A	1566	OXT	CM4-C47-C56	-2.93	121.19	127.60
2	B	1566	OXT	N11-C21-N31	-2.88	120.58	125.54
2	A	1566	OXT	C74-C64-C54	-2.82	107.66	112.36
4	A	1568	ADP	C4-C5-N7	-2.56	106.74	109.40
2	A	1566	OXT	C35-N44-C54	2.52	127.52	122.84
2	A	1566	OXT	C51-C61-N11	-2.46	119.71	123.82
2	B	1566	OXT	C74-C64-C54	-2.42	108.32	112.36
2	B	1566	OXT	C51-C61-N11	-2.41	119.81	123.82
2	B	1566	OXT	C74-N84-C94	2.35	126.77	122.59
2	B	1566	OXT	C56-C47-N43	2.34	112.56	107.66
4	A	1568	ADP	C1'-N9-C4	-2.34	122.53	126.64
2	A	1566	OXT	C56-C47-N43	2.26	112.38	107.66
4	A	1568	ADP	PA-O3A-PB	-2.23	125.19	132.83
2	B	1566	OXT	PA-O3A-PB	-2.22	125.20	132.83
6	B	1572	B3P	C3-N1-C4	-2.20	112.96	116.08
2	A	1566	OXT	CM2-C21-N11	2.17	119.53	117.14
2	B	1566	OXT	CM2-C21-N11	2.14	119.50	117.14
6	A	1571	B3P	C2-N2-C8	-2.14	113.04	116.08
6	A	1570	B3P	C3-N1-C4	-2.12	113.07	116.08
4	B	1568	ADP	PA-O3A-PB	-2.11	125.58	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1566	OXT	O3B-PB-O2B	2.10	115.68	107.64
2	B	1566	OXT	C35-N44-C54	2.10	126.74	122.84
6	B	1572	B3P	C2-N2-C8	-2.09	113.11	116.08
2	A	1566	OXT	CM2-C21-N31	2.08	120.39	117.15
4	A	1568	ADP	C2-N1-C6	2.01	122.19	118.75
4	B	1568	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1571	B3P	C6-C4-N1-C3
6	A	1571	B3P	C6-C4-C5-O4
6	A	1571	B3P	C5-C4-C6-O5
4	A	1568	ADP	O4'-C4'-C5'-O5'
2	A	1566	OXT	C47-C56-C66-C76
2	A	1566	OXT	PA-O3A-PB-O3B
6	B	1570	B3P	C6-C4-N1-C3
6	B	1570	B3P	C7-C4-N1-C3
6	B	1570	B3P	C6-C4-C5-O4
6	B	1570	B3P	C5-C4-C6-O5
6	B	1570	B3P	C9-C8-N2-C2
6	B	1570	B3P	C11-C8-N2-C2
6	B	1571	B3P	C5-C4-N1-C3
6	B	1571	B3P	C7-C4-N1-C3
6	B	1571	B3P	C6-C4-C5-O4
6	B	1571	B3P	N1-C4-C6-O5
6	B	1571	B3P	C7-C4-C6-O5
4	B	1568	ADP	O4'-C4'-C5'-O5'
6	B	1572	B3P	N1-C4-C6-O5
6	B	1572	B3P	C5-C4-C6-O5
6	B	1572	B3P	C7-C4-C6-O5
2	B	1566	OXT	C47-C56-C66-C76
2	B	1566	OXT	PA-O3A-PB-O3B
6	A	1572	B3P	N1-C4-C5-O4
6	A	1572	B3P	C6-C4-C5-O4
6	A	1572	B3P	C7-C4-C5-O4
4	B	1568	ADP	C3'-C4'-C5'-O5'
6	A	1570	B3P	C3-C1-C2-N2
4	A	1568	ADP	C3'-C4'-C5'-O5'
6	A	1570	B3P	C2-C1-C3-N1
6	B	1571	B3P	C2-C1-C3-N1

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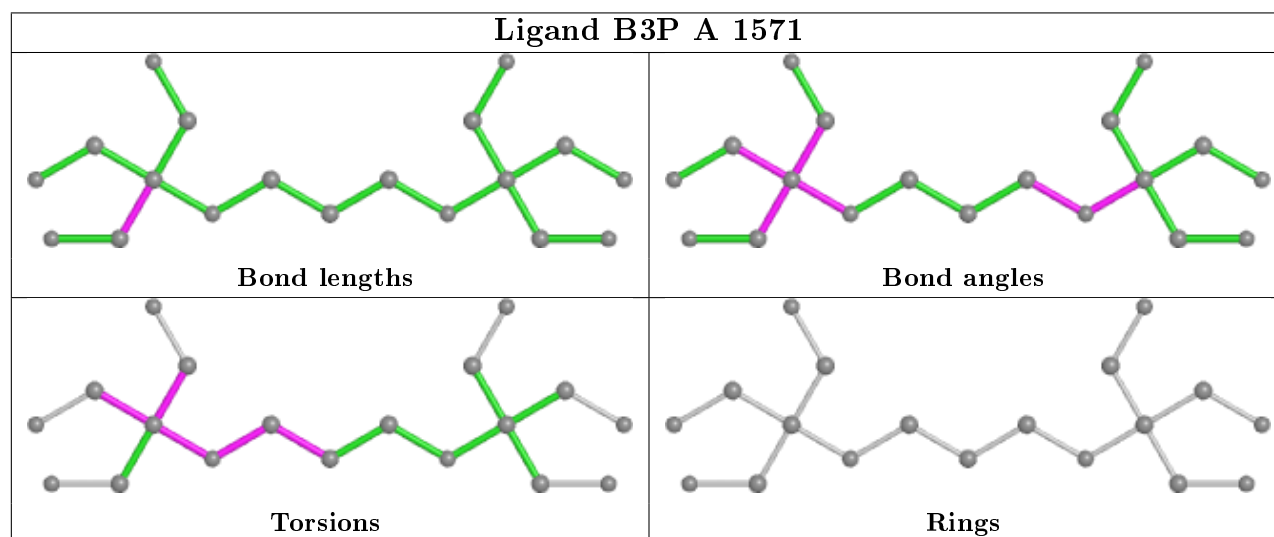
Mol	Chain	Res	Type	Atoms
5	B	1569	PGE	O1-C1-C2-O2
6	A	1571	B3P	C1-C3-N1-C4
6	A	1571	B3P	C2-C1-C3-N1
5	B	1569	PGE	O2-C3-C4-O3
6	B	1571	B3P	C7-C4-C5-O4
6	A	1572	B3P	C5-C4-C7-O6
6	B	1570	B3P	C1-C2-N2-C8
6	B	1571	B3P	C1-C3-N1-C4
6	A	1571	B3P	C7-C4-N1-C3
6	A	1572	B3P	C9-C8-N2-C2
6	B	1572	B3P	C1-C3-N1-C4
6	B	1570	B3P	C1-C3-N1-C4
6	B	1572	B3P	C10-C8-C9-O1
2	A	1566	OXT	P23-O33-P13-O13
2	B	1566	OXT	P23-O33-P13-O23
6	B	1570	B3P	C10-C8-N2-C2
6	A	1572	B3P	C11-C8-N2-C2
5	B	1569	PGE	O3-C5-C6-O4
2	A	1566	OXT	P23-O33-P13-O23
2	B	1566	OXT	P23-O33-P13-O13
5	A	1569	PGE	O1-C1-C2-O2
6	A	1572	B3P	C2-C1-C3-N1
6	A	1570	B3P	C11-C8-N2-C2
2	A	1566	OXT	C35-C25-S15-C40
2	B	1566	OXT	C35-C25-S15-C40
2	A	1566	OXT	PA-O3A-PB-O2B
2	B	1566	OXT	PA-O3A-PB-O2B
6	B	1572	B3P	N2-C8-C9-O1
6	A	1572	B3P	N1-C4-C7-O6
5	B	1569	PGE	C1-C2-O2-C3
2	A	1566	OXT	PA-O3A-PB-O1B
2	B	1566	OXT	PA-O3A-PB-O1B
6	B	1570	B3P	C7-C4-C5-O4
6	B	1570	B3P	C11-C8-C9-O1
6	B	1572	B3P	C11-C8-C9-O1
6	A	1572	B3P	C6-C4-C7-O6
6	A	1572	B3P	O3-C11-C8-C10
5	A	1569	PGE	C4-C3-O2-C2
5	B	1569	PGE	C4-C3-O2-C2

There are no ring outliers.

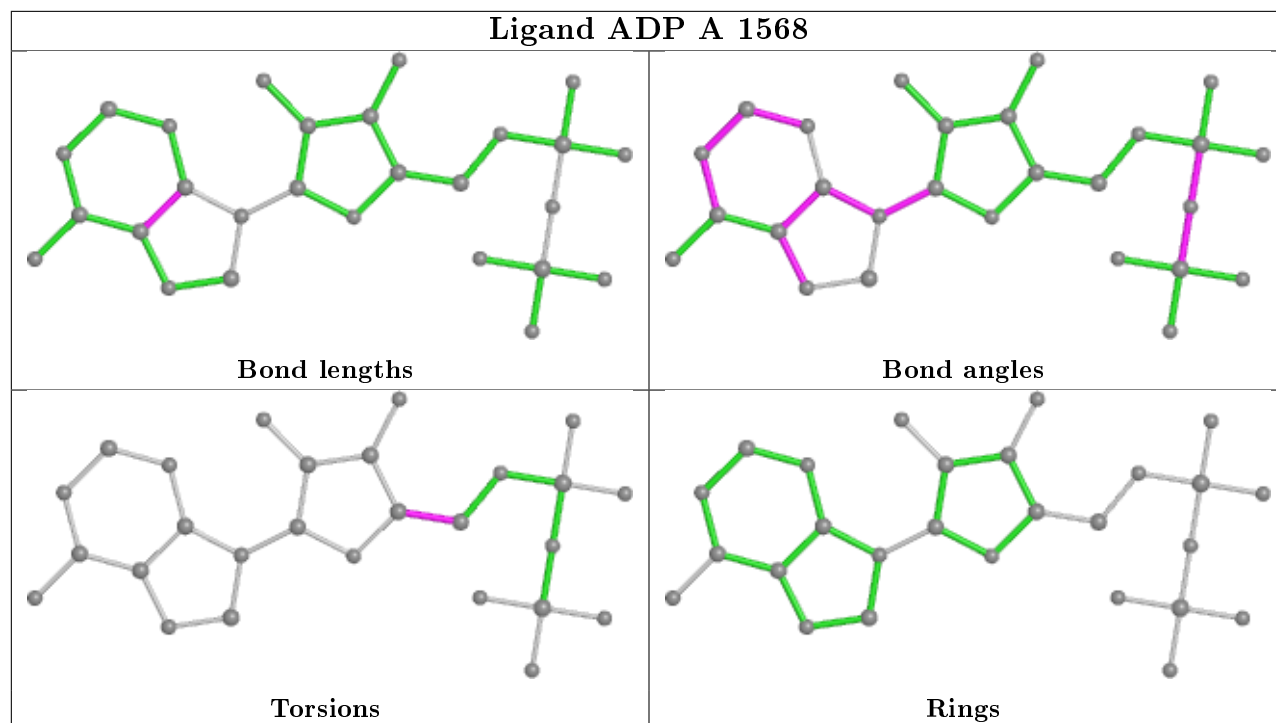
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1571	B3P	1	0
2	A	1566	OXT	2	0
6	B	1570	B3P	3	0
2	B	1566	OXT	5	0

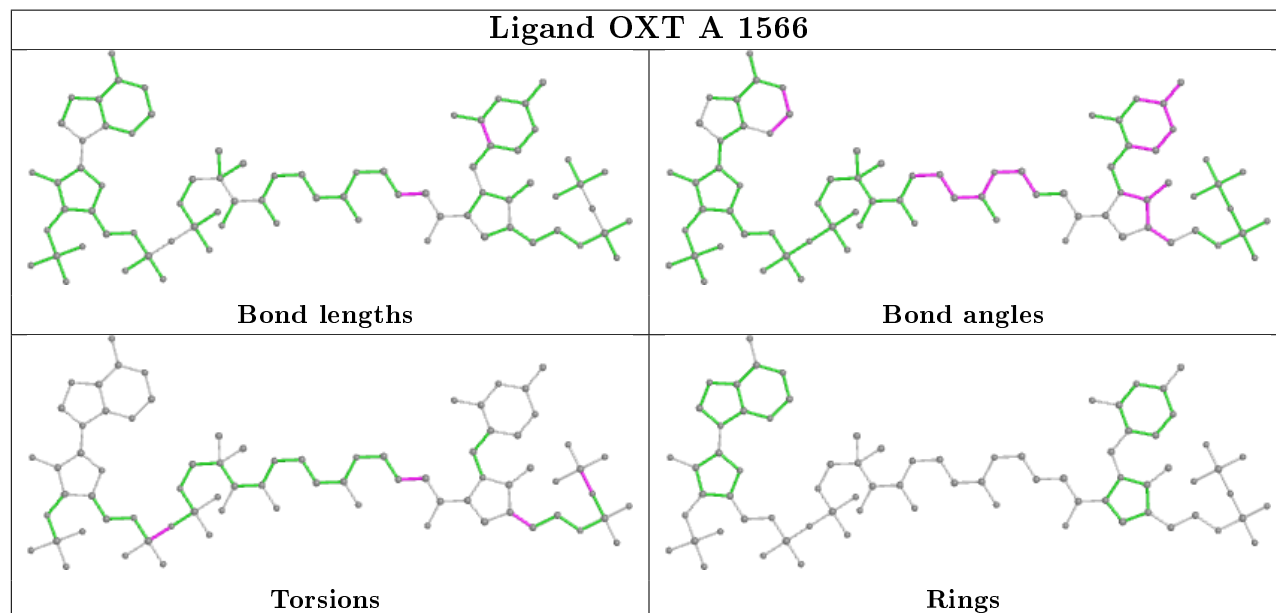
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

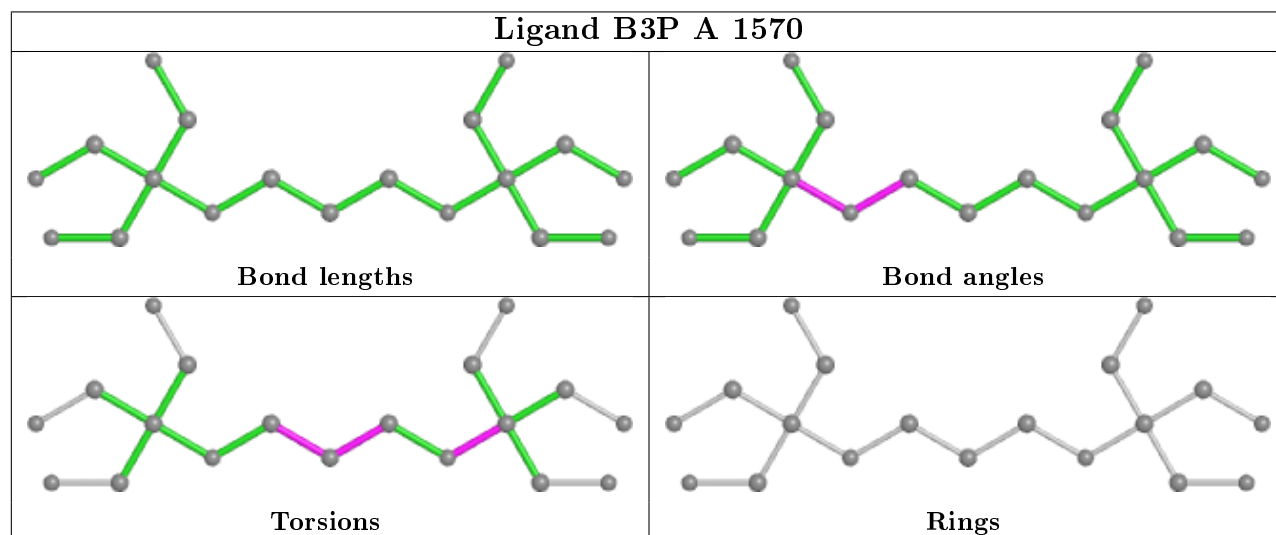
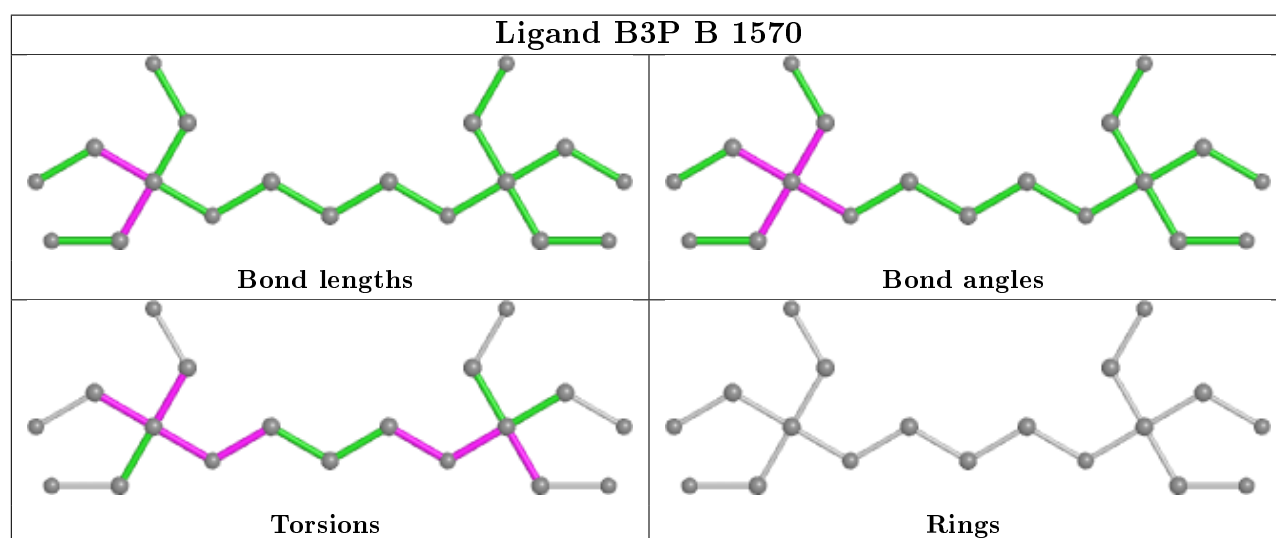
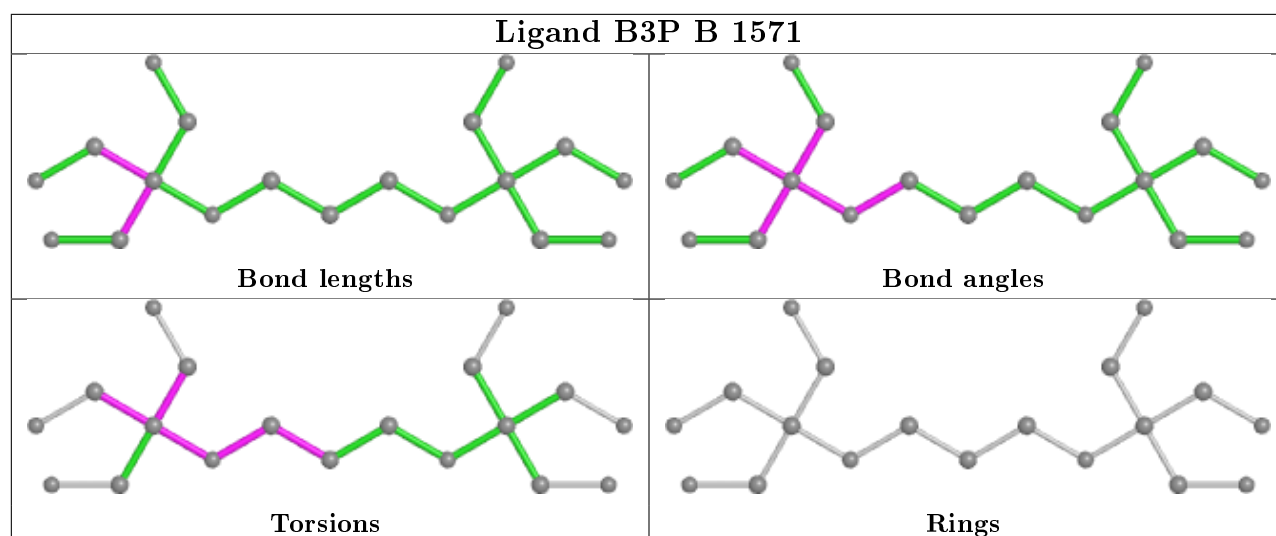


Ligand ADP A 1568

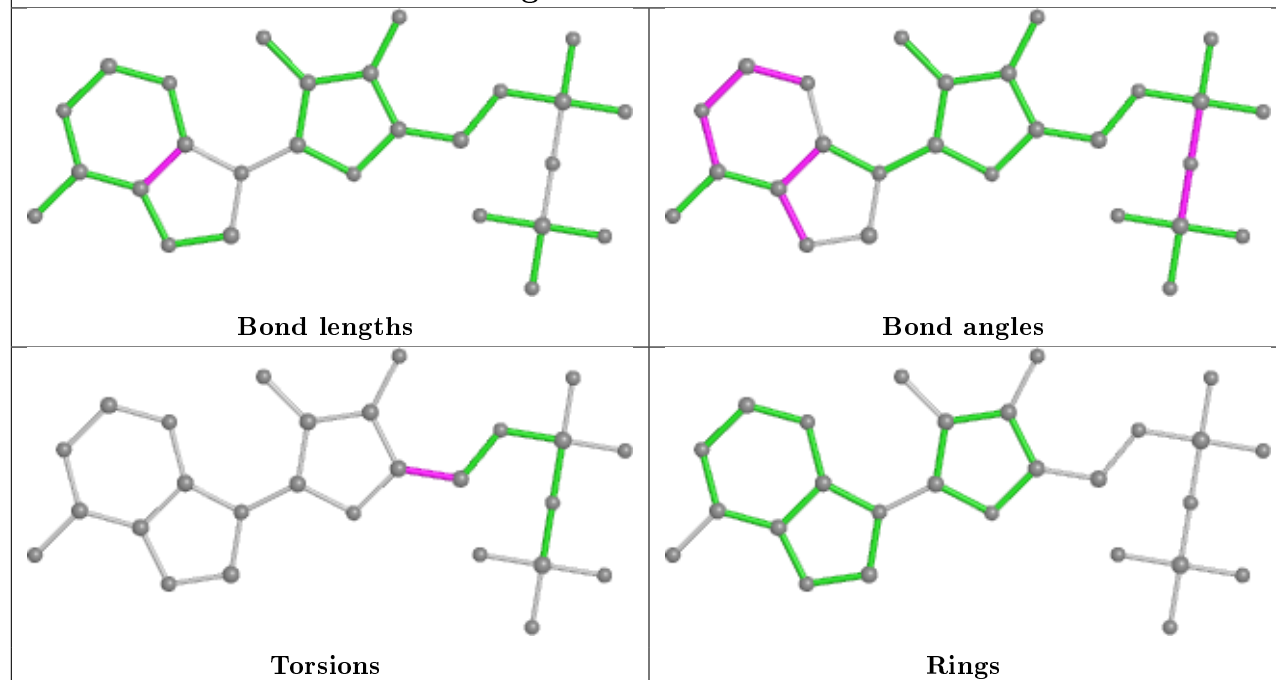


Ligand OXT A 1566

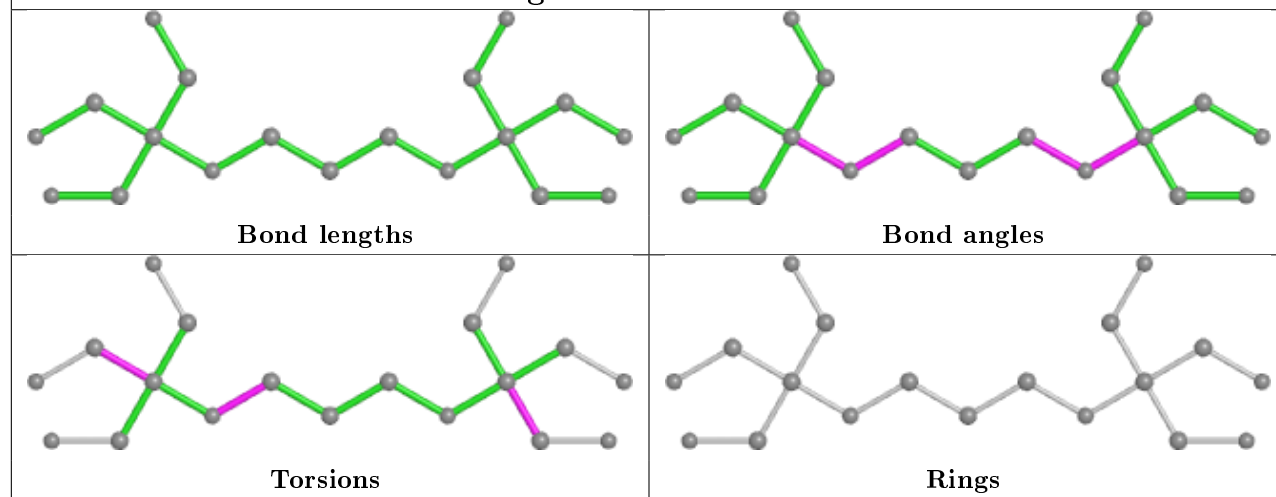


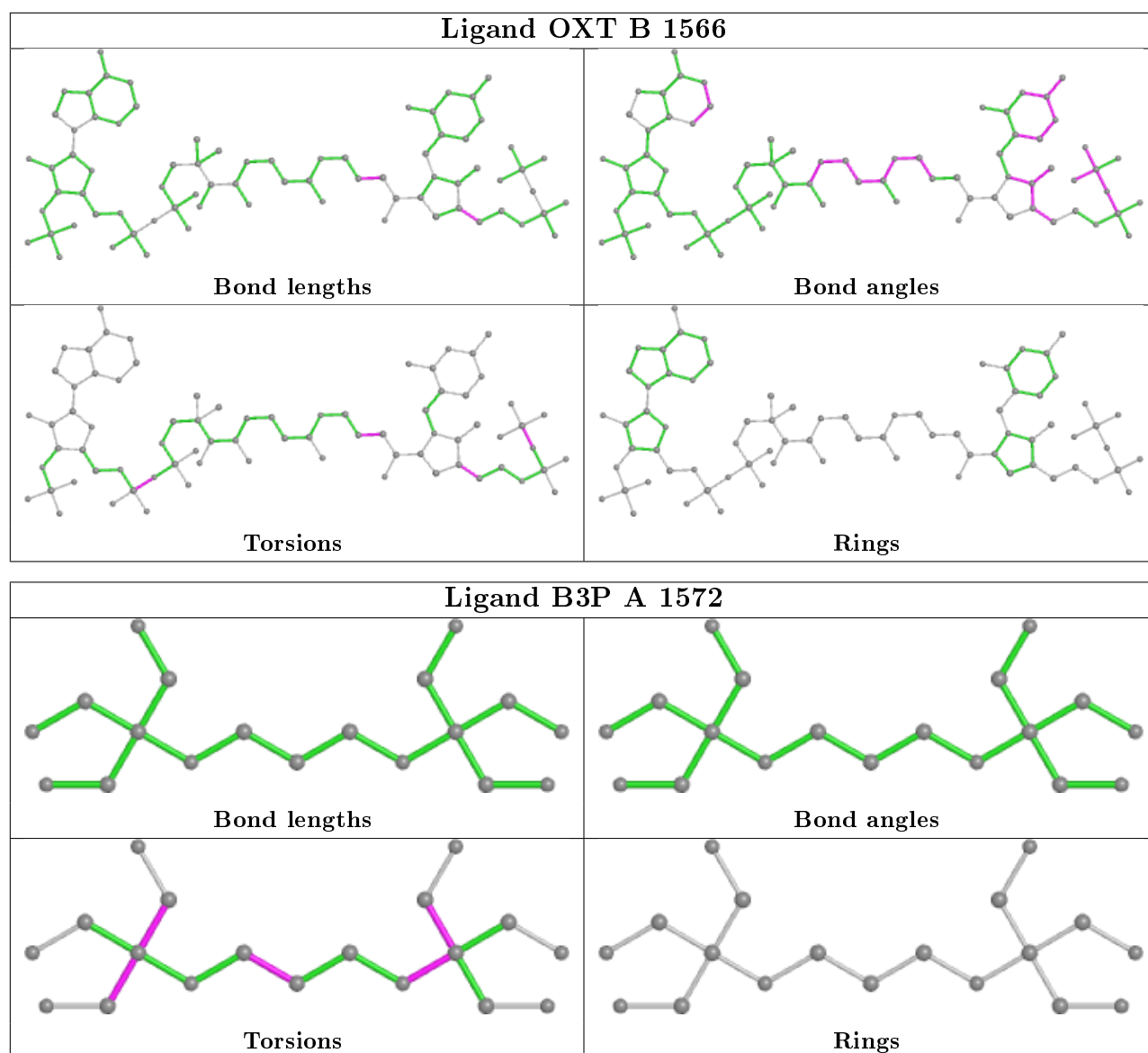


Ligand ADP B 1568



Ligand B3P B 1572





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	559/568 (98%)	-0.06	5 (0%)	84 82	19, 24, 32, 48	0
1	B	559/568 (98%)	-0.08	4 (0%)	87 86	20, 24, 32, 50	0
All	All	1118/1136 (98%)	-0.07	9 (0%)	86 84	19, 24, 32, 50	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	VAL	8.0
1	B	7	VAL	5.8
1	A	565	VAL	4.2
1	B	565	VAL	3.4
1	A	127[A]	ASN	2.9
1	A	564	LYS	2.8
1	B	564	LYS	2.6
1	A	128	VAL	2.4
1	B	293	LYS	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 carbohydrates 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,

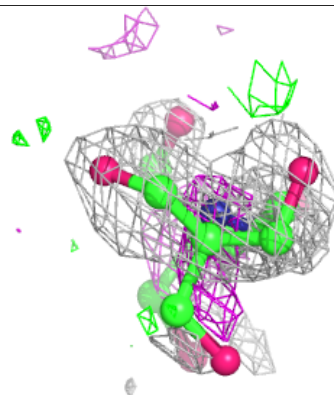
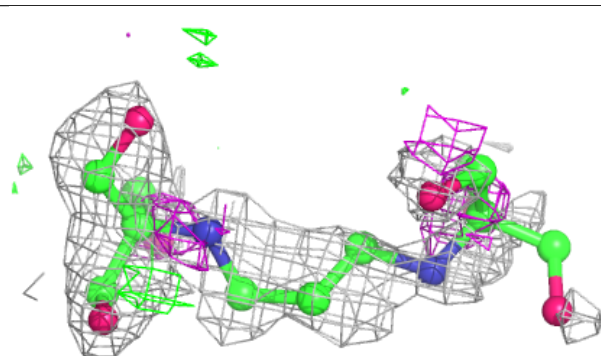
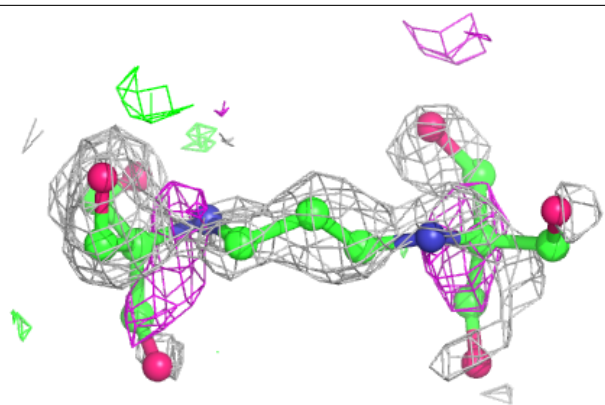
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	B3P	A	1572	19/19	0.46	0.35	58,62,68,69	0
6	B3P	B	1570	19/19	0.50	0.44	69,74,81,81	0
6	B3P	A	1571	19/19	0.64	0.39	54,61,69,69	0
6	B3P	B	1572	19/19	0.65	0.30	37,45,55,55	0
6	B3P	B	1571	19/19	0.74	0.28	47,54,65,65	0
5	PGE	B	1569	10/10	0.76	0.21	50,51,52,52	0
6	B3P	A	1570	19/19	0.86	0.24	37,46,57,58	0
5	PGE	A	1569	10/10	0.91	0.11	41,42,43,43	0
2	OXT	B	1566	76/76	0.94	0.19	15,30,33,35	50
2	OXT	A	1566	76/76	0.95	0.15	13,24,28,32	50
4	ADP	B	1568	27/27	0.98	0.08	13,15,16,17	0
4	ADP	A	1568	27/27	0.98	0.08	12,15,17,17	0
3	MG	B	1567	1/1	0.99	0.07	13,13,13,13	0
3	MG	A	1567	1/1	0.99	0.07	11,11,11,11	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.

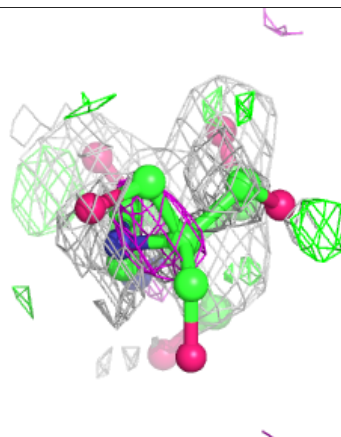
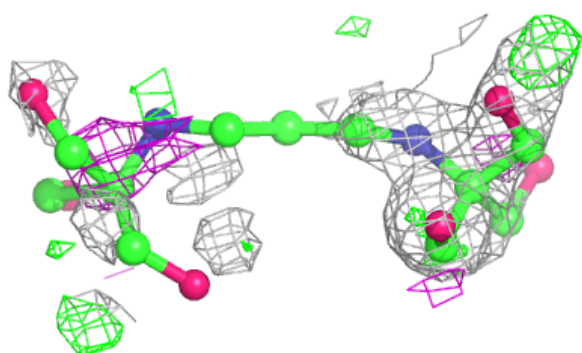
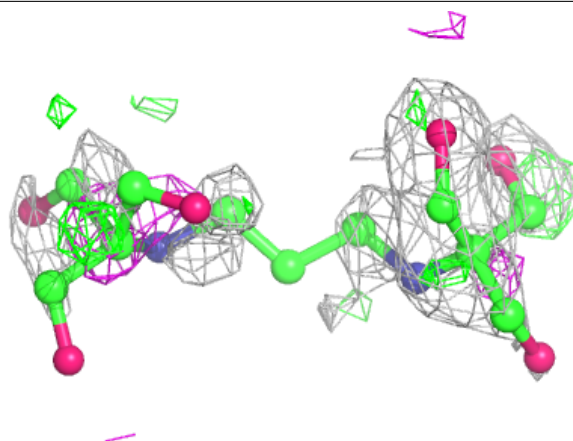
Electron density around B3P A 1572:

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

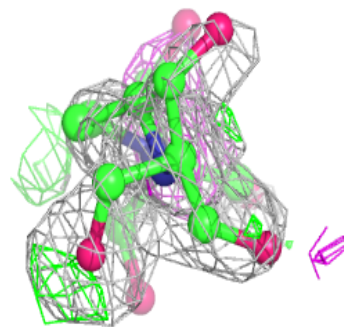
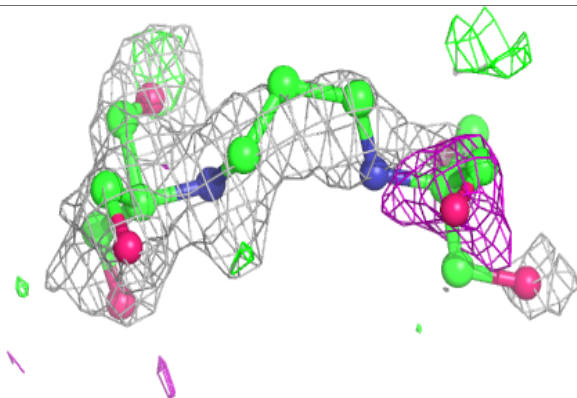
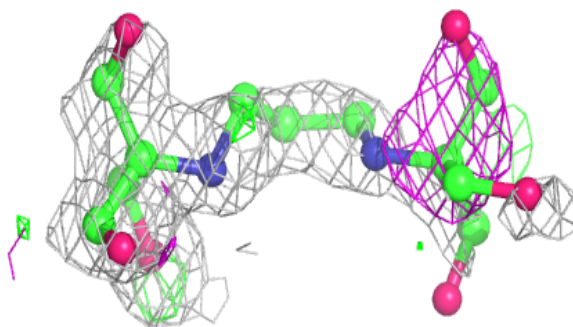


Electron density around B3P B 1570:

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

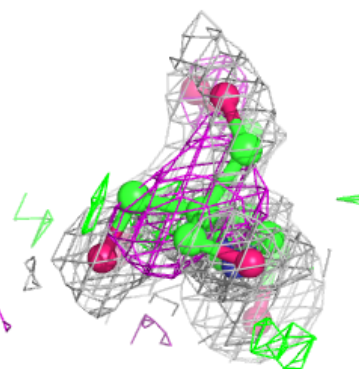
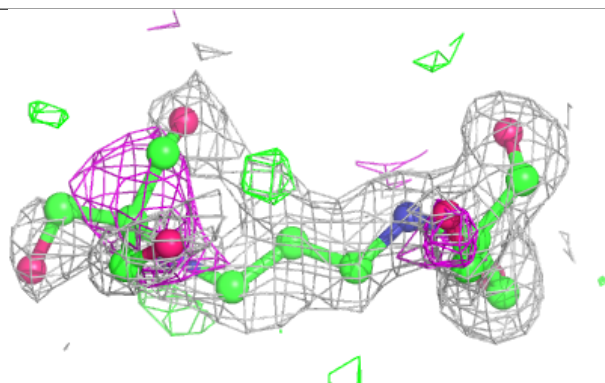
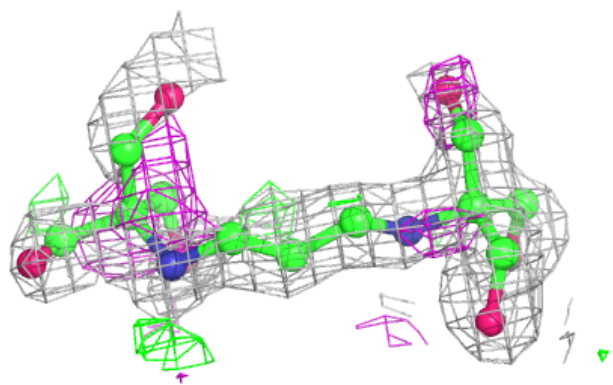
**Electron density around B3P A 1571:**

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

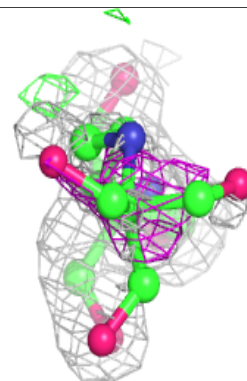
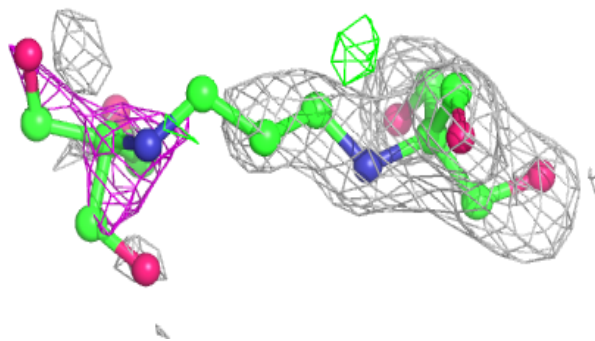
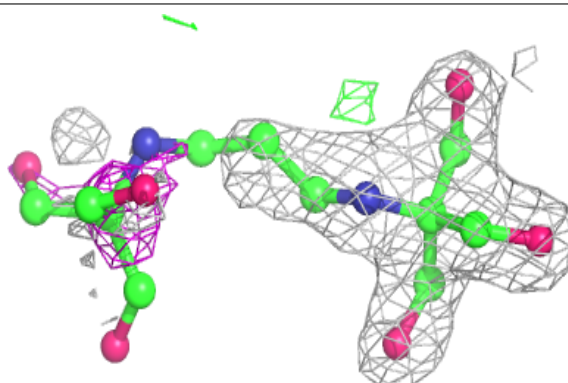


Electron density around B3P B 1572:

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

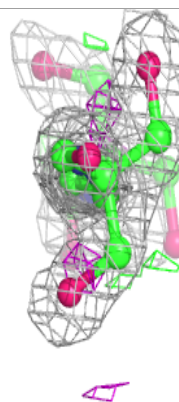
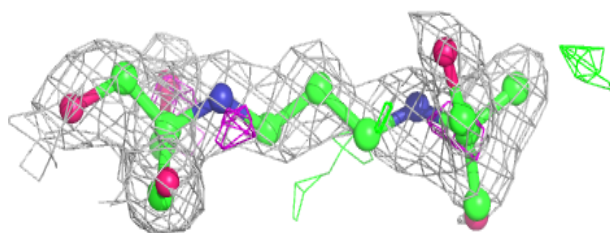
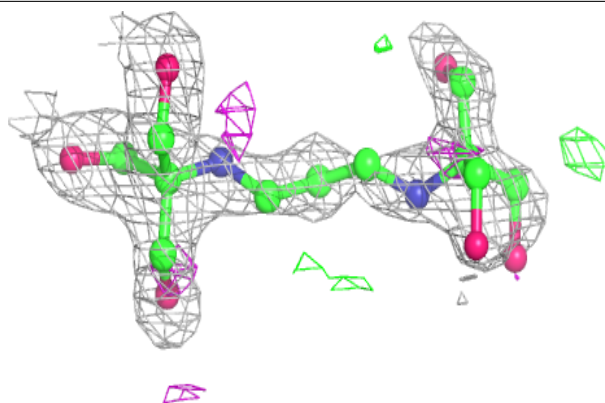
**Electron density around B3P B 1571:**

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

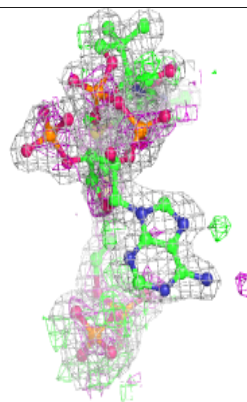
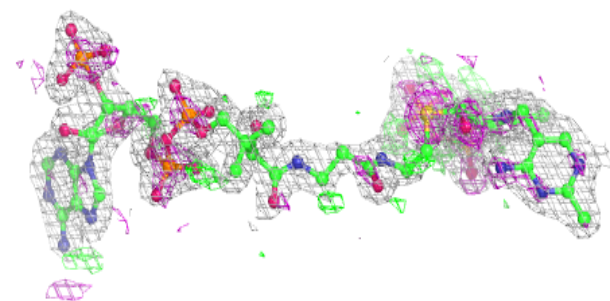
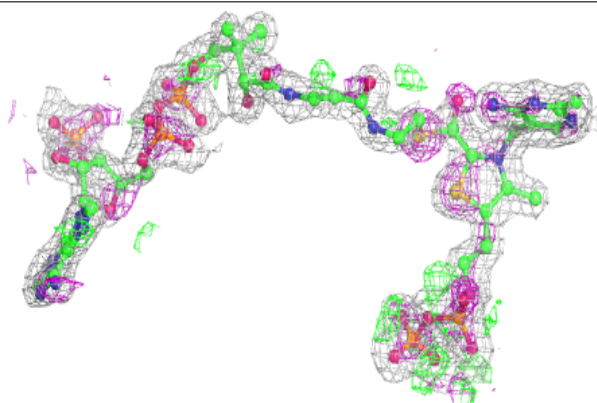


Electron density around B3P A 1570:

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

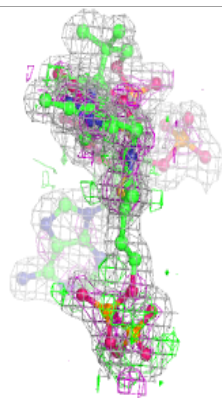
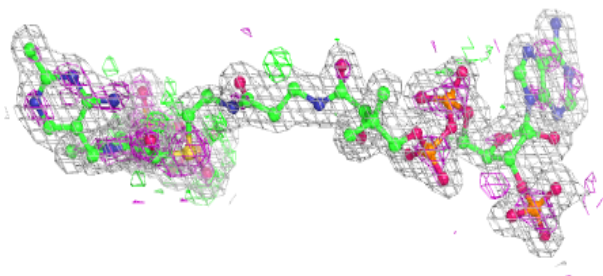
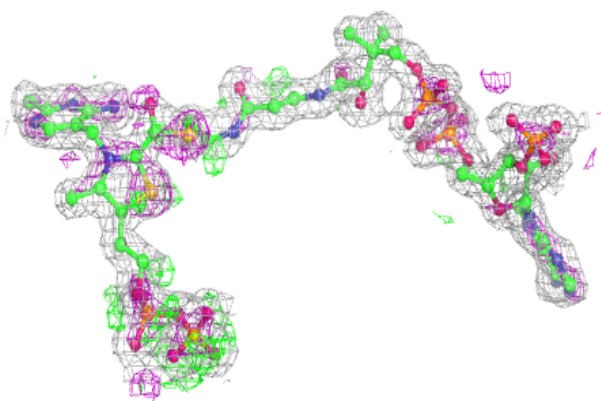
**Electron density around OXT B 1566:**

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

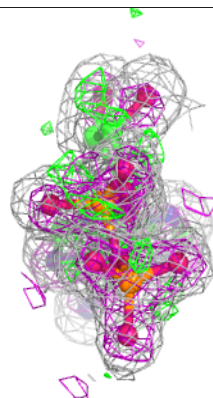
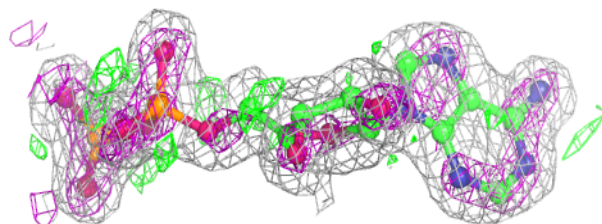
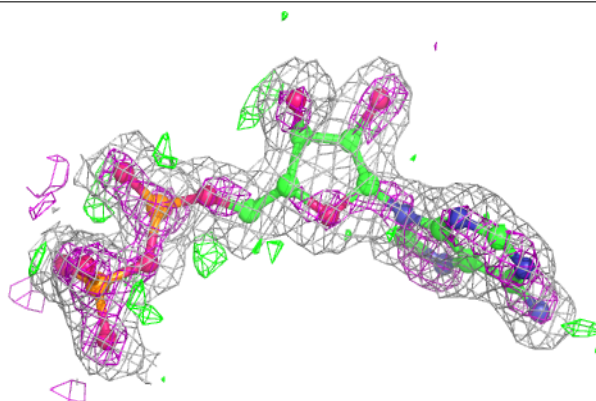


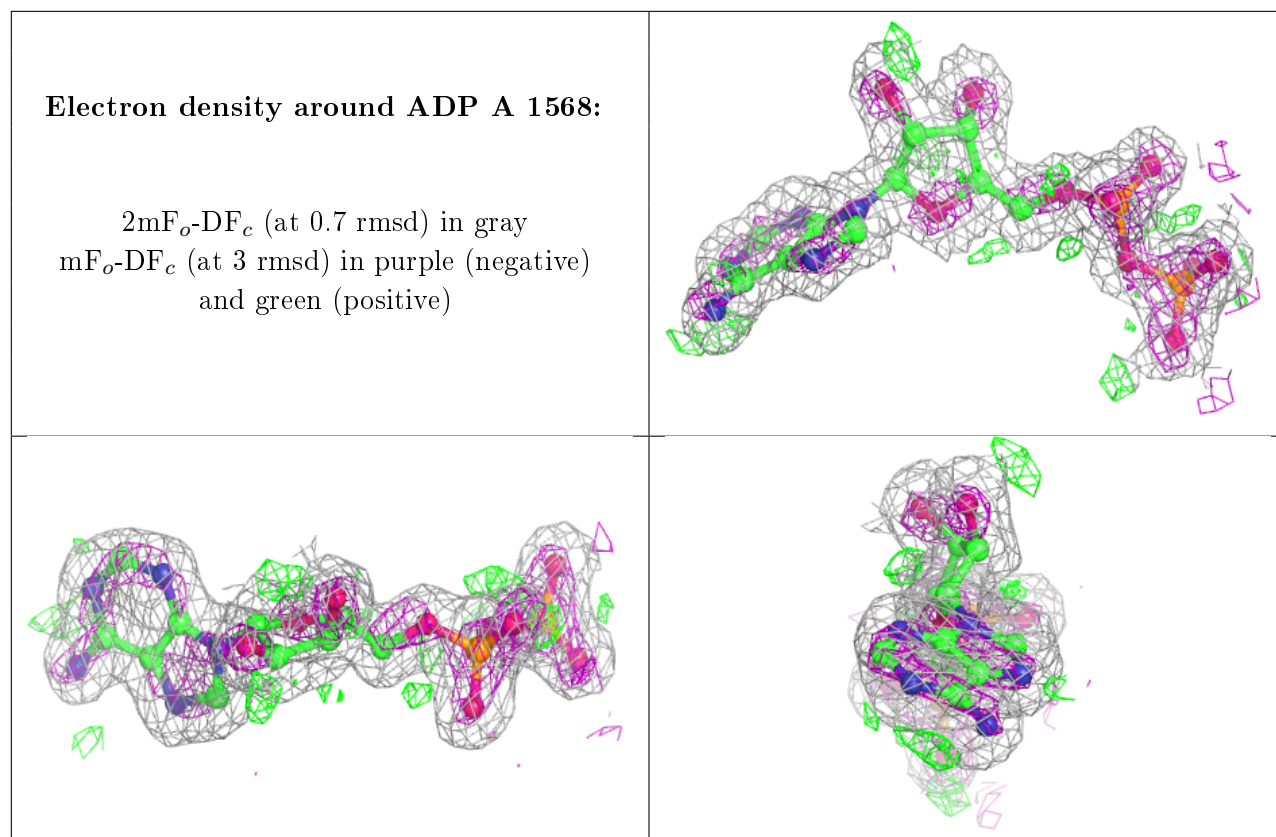
Electron density around OXT A 1566:

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

**Electron density around ADP B 1568:**

$2mF_o-DF_c$ (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.