Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 01:48 AM EDT

PDB ID	:	7LOM
Title	:	Ornithine Aminotransferase (OAT) soaked with its inactivator - (1S,3S)-3-amino-4-(difluoromethylene)cyclohexene-1-carboxylic acid
Authors	:	Butrin, A.; Zhu, W.; Liu, D.; Silverman, R.
Deposited on	:	2021-02-10
Resolution	:	2.10 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:

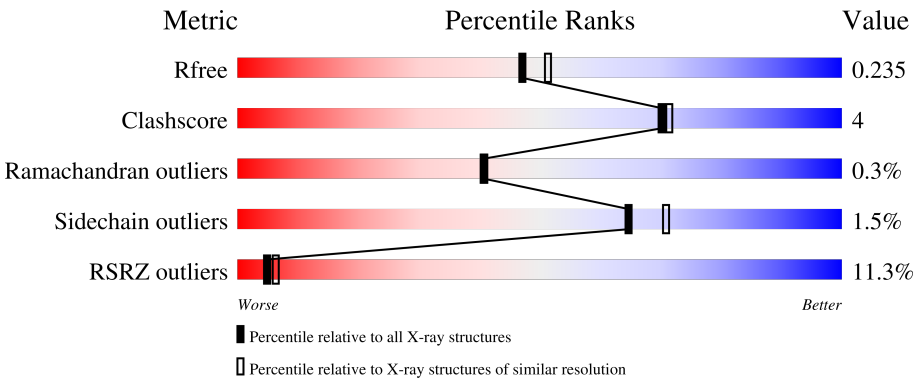
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	404	8% 87% 12% •
1	B	404	17% 91% 8%
1	C	404	9% 92% 6% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Y8P	B	502	X	-	-	-

2 Entry composition (i)

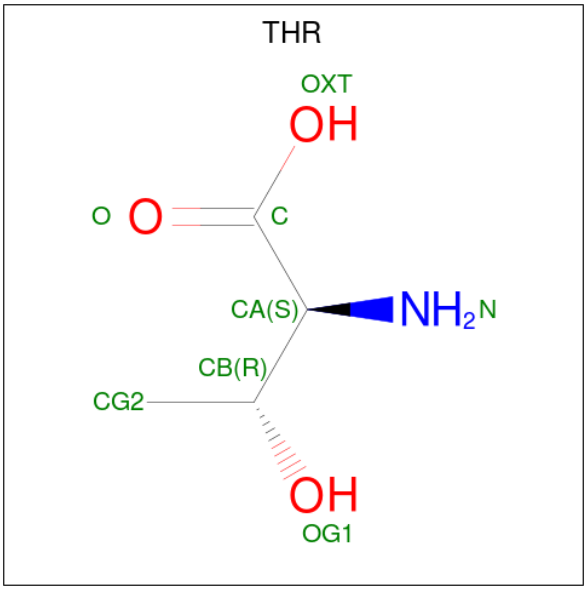
There are 5 unique types of molecules in this entry. The entry contains 10020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ornithine aminotransferase, mitochondrial.

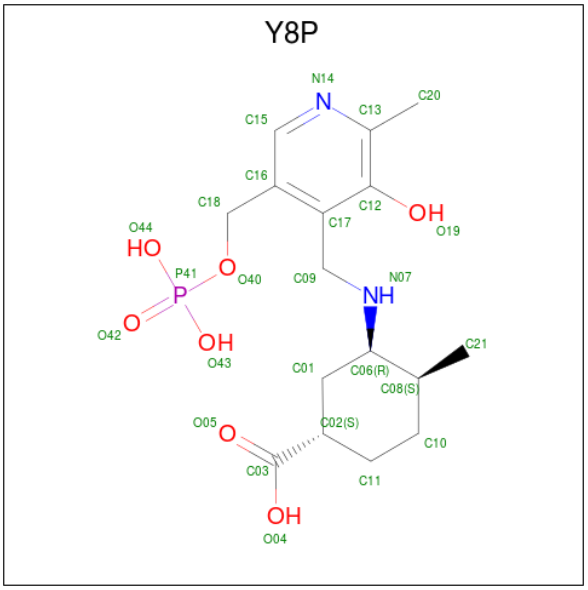
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3150	2024	531	583	12	0	0	0
1	B	402	3150	2024	531	583	12	0	0	0
1	C	402	3150	2024	531	583	12	0	0	0

- Molecule 2 is THREONINE (three-letter code: THR) (formula: $C_4H_9NO_3$).



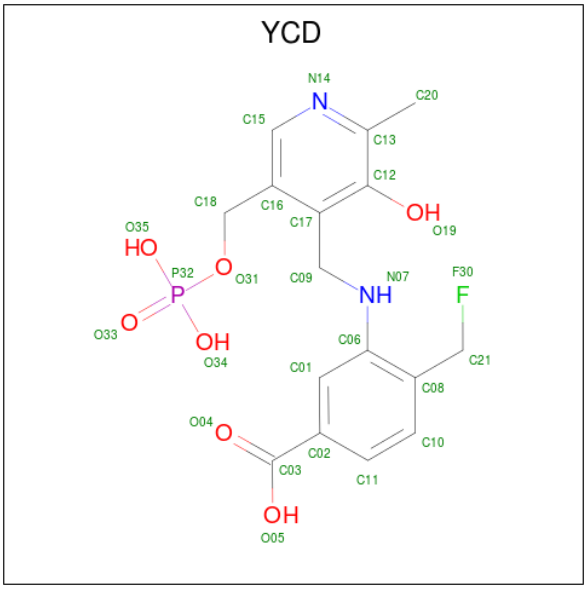
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	7	4	1	2	0	0
2	B	1	7	4	1	2	0	0
2	C	1	7	4	1	2	0	0

- Molecule 3 is (3 {S},4 {S})-4-methyl-3-[[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methylamino]cyclohexene-1-carboxylic acid (three-letter code: Y8P) (formula: $C_{16}H_{25}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	26	16	2	7	1	0	0
			Total	C	N	O	P		
3	B	1	26	16	2	7	1	0	0

- Molecule 4 is (4 {R})-4-(fluoranylmethyl)-3-[[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methylamino]cyclohexene-1-carboxylic acid (three-letter code: YCD) (formula: $C_{16}H_{18}FN_2O_7P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
4	C	1	27	16	1	2	7	1	0	0

- Molecule 5 is water.

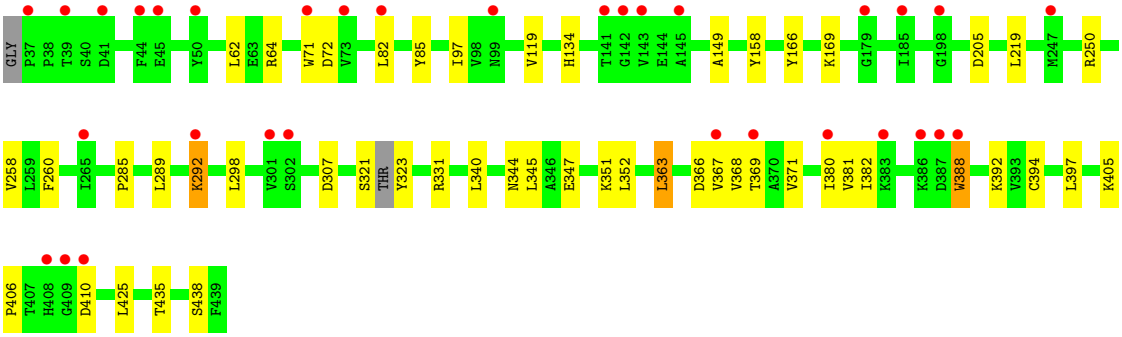
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	158	158	158	0	0
			Total	O		
5	B	131	131	131	0	0
			Total	O		
5	C	181	181	181	0	0

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.

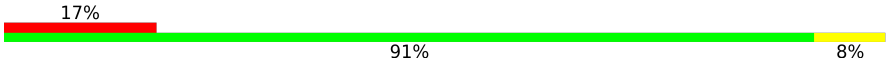
• Molecule 1: Ornithine aminotransferase, mitochondrial

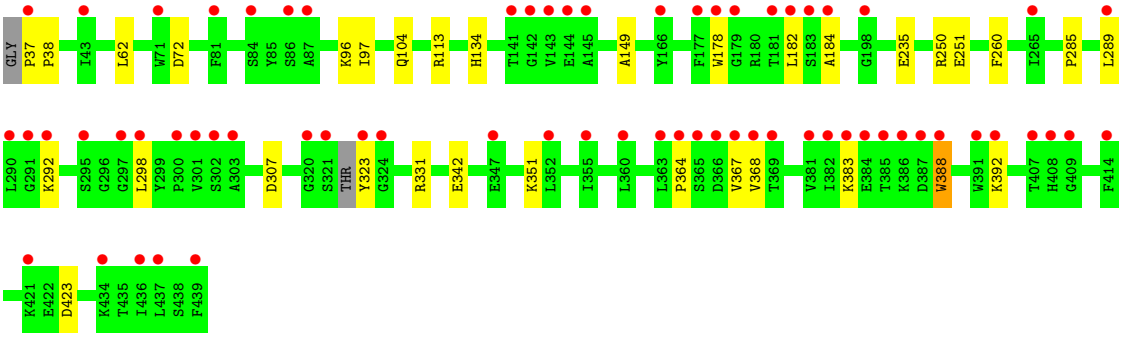
Chain A:



• Molecule 1: Ornithine aminotransferase, mitochondrial

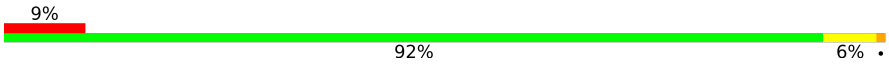
Chain B:

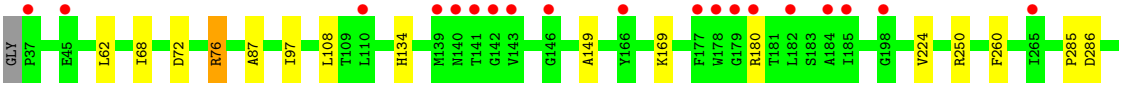


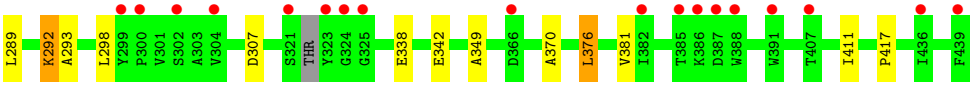


• Molecule 1: Ornithine aminotransferase, mitochondrial

Chain C:






L289
K292
A293
L298
Y299
P300
V301
S302
A303
V304
D307
S321
THR
Y323
G324
G325
E338
E342
A349
D366
A370
L376
V381
I382
T385
K386
D387
W388
W391
T407
I411
P417
I436
F439

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.61Å 115.61Å 186.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.11 – 2.10 44.11 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.11-2.10) 98.4 (44.11-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.235 0.200 , 0.235	Depositor DCC
R_{free} test set	4101 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10020	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: YCD, Y8P

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	0.25	0/3223	0.44	0/4374
1	B	0.25	0/3223	0.44	0/4374
1	C	0.25	0/3223	0.44	0/4374
All	All	0.25	0/9669	0.44	0/13122

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	3150	0	3152	29	2
1	B	3150	0	3153	19	2
1	C	3150	0	3155	17	0
2	A	7	0	5	0	2
2	B	7	0	5	0	0
2	C	7	0	5	0	2
3	A	26	0	0	1	0
3	B	26	0	0	2	0
4	C	27	0	0	2	0
5	A	158	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	131	0	0	2	0
5	C	181	0	0	0	0
All	All	10020	0	9475	68	4

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 (68) 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:37:PRO:HB2	1:B:38:PRO:HD3	1.48	0.93
1:B:134:HIS:HB2	1:B:307:ASP:HA	1.68	0.75
1:A:134:HIS:HB2	1:A:307:ASP:HA	1.77	0.65
1:A:347:GLU:HG2	1:A:351:LYS:HE2	1.80	0.63
1:B:37:PRO:HB2	1:B:38:PRO:CD	2.27	0.61
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.83	0.60
1:A:344:ASN:ND2	1:A:347:GLU:OE1	2.35	0.60
1:A:62:LEU:HA	1:A:72:ASP:HA	1.84	0.59
1:A:367:VAL:HG13	1:A:388:TRP:HH2	1.68	0.59
1:C:134:HIS:HB2	1:C:307:ASP:HA	1.86	0.57
1:B:149:ALA:HB2	1:B:289:LEU:HD21	1.87	0.56
1:A:367:VAL:HG12	1:A:368:VAL:HG23	1.87	0.56
1:A:363:LEU:HD23	1:A:368:VAL:HG21	1.87	0.56
1:A:82:LEU:HD23	1:A:85:TYR:H	1.71	0.56
1:C:349:ALA:HA	1:C:376:LEU:HD22	1.87	0.56
1:A:340:LEU:HD23	1:A:345:LEU:HD12	1.89	0.55
3:B:502:Y8P:O19	3:B:502:Y8P:N07	2.39	0.54
1:A:405:LYS:HG3	1:A:406:PRO:HD2	1.90	0.54
1:A:119:VAL:HG11	1:A:331:ARG:HG2	1.90	0.53
1:A:219:LEU:HD22	1:A:258:VAL:HG21	1.90	0.53
1:C:149:ALA:HB2	1:C:289:LEU:HD21	1.89	0.53
1:A:371:VAL:HG22	1:A:380:ILE:HG22	1.91	0.53
1:B:423:ASP:N	1:B:423:ASP:OD1	2.42	0.53
1:A:367:VAL:HG13	1:A:388:TRP:CH2	2.43	0.52
1:C:62:LEU:HA	1:C:72:ASP:HA	1.92	0.52
1:C:87:ALA:HB2	1:C:292:LYS:HG3	1.91	0.51
1:C:97:ILE:HG22	1:C:298:LEU:HD22	1.92	0.50
1:A:64:ARG:HB3	1:A:71:TRP:HB2	1.92	0.50
1:C:250:ARG:O	1:C:250:ARG:HD3	2.12	0.50
1:A:97:ILE:HG22	1:A:298:LEU:HD22	1.94	0.49
1:C:370:ALA:HB3	1:C:381:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ARG:HH21	1:B:285:PRO:HA	1.78	0.48
1:B:364:PRO:HG2	1:B:367:VAL:HG22	1.95	0.48
1:C:292:LYS:HE3	4:C:502:YCD:N07	2.28	0.48
1:B:97:ILE:HG22	1:B:298:LEU:HD22	1.95	0.48
1:B:388:TRP:HA	1:B:392:LYS:HD2	1.94	0.48
3:A:502:Y8P:O19	3:A:502:Y8P:N07	2.46	0.47
1:C:250:ARG:HH21	1:C:285:PRO:HA	1.79	0.47
1:B:113:ARG:NH1	5:B:608:HOH:O	2.48	0.45
1:B:235:GLU:HG2	3:B:502:Y8P:C03	2.46	0.45
4:C:502:YCD:N07	4:C:502:YCD:O19	2.49	0.45
1:B:96:LYS:NZ	1:B:342:GLU:OE2	2.49	0.45
1:C:68:ILE:HA	1:C:417:PRO:HG2	1.98	0.45
1:A:250:ARG:O	1:A:250:ARG:HD3	2.17	0.44
1:A:394:CYS:SG	1:A:406:PRO:HD3	2.57	0.44
1:B:178:TRP:CZ2	1:B:184:ALA:HA	2.53	0.44
1:A:250:ARG:HH21	1:A:285:PRO:HA	1.83	0.43
1:A:388:TRP:HA	1:A:392:LYS:HD2	2.00	0.43
1:B:104:GLN:HB2	1:B:331:ARG:HG3	2.01	0.43
1:C:381:VAL:HG22	1:C:411:ILE:HG12	2.01	0.43
1:A:397:LEU:HG	1:A:435:THR:HG21	2.01	0.43
1:B:367:VAL:HG23	1:B:368:VAL:HG23	2.01	0.43
1:A:435:THR:O	1:A:438:SER:OG	2.33	0.42
1:C:292:LYS:HB3	1:C:293:ALA:H	1.56	0.42
1:A:64:ARG:NH1	5:A:611:HOH:O	2.48	0.42
1:B:367:VAL:HB	1:B:388:TRP:CH2	2.55	0.42
1:B:250:ARG:O	1:B:250:ARG:HD3	2.20	0.41
1:C:338:GLU:O	1:C:342:GLU:HG2	2.20	0.41
1:A:382:ILE:N	1:A:410:ASP:O	2.52	0.41
1:A:369:THR:OG1	1:A:381:VAL:HG13	2.21	0.41
1:C:169:LYS:HB2	1:C:224:VAL:HA	2.02	0.41
1:B:251:GLU:OE2	5:B:601:HOH:O	2.22	0.41
1:C:250:ARG:HH22	1:C:286:ASP:CG	2.24	0.41
1:A:158:TYR:OH	1:A:166:TYR:HA	2.21	0.41
1:A:169:LYS:HD3	1:A:205:ASP:OD2	2.21	0.40
1:A:352:LEU:HB3	1:A:425:LEU:HD22	2.03	0.40
1:B:62:LEU:HA	1:B:72:ASP:HA	2.03	0.40
1:C:72:ASP:OD1	1:C:76:ARG:N	2.54	0.40

All (4) 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:323:TYR:N	2:C:501:THR:O[2_444]	1.30	0.90
1:A:321:SER:C	2:A:501:THR:N[6_554]	1.43	0.77
1:A:323:TYR:N	2:A:501:THR:C[6_554]	1.43	0.77
1:B:323:TYR:CA	2:C:501:THR:O[2_444]	1.79	0.41

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	398/404 (98%)	381 (96%)	16 (4%)	1 (0%)	41	41
1	B	398/404 (98%)	381 (96%)	15 (4%)	2 (0%)	29	26
1	C	398/404 (98%)	381 (96%)	17 (4%)	0	100	100
All	All	1194/1212 (98%)	1143 (96%)	48 (4%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	LYS
1	B	292	LYS
1	B	383	LYS

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	336/337 (100%)	331 (98%)	5 (2%)	65	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	336/337 (100%)	332 (99%)	4 (1%)	71	77
1	C	336/337 (100%)	330 (98%)	6 (2%)	59	65
All	All	1008/1011 (100%)	993 (98%)	15 (2%)	65	71

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

Mol	Chain	Res	Type
1	A	260	PHE
1	A	292	LYS
1	A	363	LEU
1	A	366	ASP
1	A	388	TRP
1	B	182	LEU
1	B	260	PHE
1	B	351	LYS
1	B	388	TRP
1	C	76	ARG
1	C	108	LEU
1	C	180	ARG
1	C	260	PHE
1	C	292	LYS
1	C	376	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	Y8P	A	502	2,1	27,27,27	1.63	5 (18%)	33,39,39	2.48	11 (33%)
2	THR	C	501	4,1	5,6,7	1.23	1 (20%)	6,7,9	1.10	0
2	THR	B	501	3,1	5,6,7	0.71	0	6,7,9	1.45	1 (16%)
2	THR	A	501	3	5,6,7	0.75	0	6,7,9	1.22	0
4	YCD	C	502	2	27,28,28	4.82	10 (37%)	36,40,40	1.39	5 (13%)
3	Y8P	B	502	2,1	27,27,27	1.71	4 (14%)	33,39,39	2.81	9 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y8P	A	502	2,1	-	2/15/28/28	0/2/2/2
2	THR	C	501	4,1	-	1/5/6/8	-
2	THR	B	501	3,1	-	1/5/6/8	-
2	THR	A	501	3	-	1/5/6/8	-
4	YCD	C	502	2	-	4/15/17/17	0/2/2/2
3	Y8P	B	502	2,1	3/3/5/6	7/15/28/28	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	YCD	C01-C02	11.26	1.56	1.39
4	C	502	YCD	C11-C10	11.05	1.58	1.38
4	C	502	YCD	C06-C08	10.29	1.53	1.40
4	C	502	YCD	C11-C02	9.71	1.55	1.39
4	C	502	YCD	C01-C06	8.66	1.53	1.39
3	B	502	Y8P	C09-C17	5.35	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	YCD	C10-C08	5.21	1.48	1.39
3	A	502	Y8P	C09-C17	4.70	1.57	1.51
4	C	502	YCD	C09-C17	4.37	1.57	1.51
4	C	502	YCD	C06-N07	-4.19	1.26	1.37
4	C	502	YCD	O19-C12	3.48	1.45	1.37
3	A	502	Y8P	C20-C13	3.30	1.56	1.50
3	B	502	Y8P	C20-C13	3.24	1.55	1.50
3	A	502	Y8P	C21-C08	2.88	1.60	1.53
3	B	502	Y8P	C21-C08	2.86	1.60	1.53
3	B	502	Y8P	C06-N07	2.73	1.53	1.47
3	A	502	Y8P	C06-N07	2.38	1.52	1.47
2	C	501	THR	O-C	2.32	1.29	1.19
4	C	502	YCD	C02-C03	2.22	1.54	1.49
3	A	502	Y8P	P41-O40	2.01	1.66	1.60

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	Y8P	C01-C02-C11	8.16	120.87	109.86
3	B	502	Y8P	C21-C08-C10	8.13	125.93	111.04
3	A	502	Y8P	C21-C08-C10	7.83	125.38	111.04
3	A	502	Y8P	C01-C02-C11	6.22	118.26	109.86
3	B	502	Y8P	C11-C02-C03	5.75	122.50	111.32
3	B	502	Y8P	C10-C11-C02	4.81	119.25	111.18
3	A	502	Y8P	C11-C02-C03	4.70	120.45	111.32
3	B	502	Y8P	C01-C06-N07	4.13	121.29	112.11
4	C	502	YCD	C10-C11-C02	-3.21	117.05	120.78
3	A	502	Y8P	C10-C11-C02	3.20	116.55	111.18
4	C	502	YCD	C11-C10-C08	-2.89	117.58	121.39
4	C	502	YCD	C10-C08-C06	2.89	121.18	118.32
3	B	502	Y8P	C09-C17-C16	2.86	122.89	119.71
3	A	502	Y8P	C09-N07-C06	-2.77	109.07	114.90
3	A	502	Y8P	C01-C06-N07	2.76	118.25	112.11
3	B	502	Y8P	C01-C02-C03	2.69	116.60	110.99
3	A	502	Y8P	C17-C09-N07	-2.67	104.43	111.78
3	A	502	Y8P	C09-C17-C16	2.66	122.66	119.71
3	A	502	Y8P	C01-C02-C03	2.49	116.19	110.99
4	C	502	YCD	C21-C08-C10	-2.35	116.32	120.86
3	A	502	Y8P	O04-C03-C02	2.31	120.25	114.21
3	B	502	Y8P	C11-C10-C08	2.31	115.68	112.22
4	C	502	YCD	O05-C03-C02	2.14	120.41	114.85
3	A	502	Y8P	C20-C13-C12	-2.14	118.25	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	Y8P	C09-N07-C06	-2.13	110.43	114.90
2	B	501	THR	CB-CA-C	-2.01	108.56	111.77

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	502	Y8P	C02
3	B	502	Y8P	C06
3	B	502	Y8P	C08

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	THR	O-C-CA-CB
2	C	501	THR	O-C-CA-CB
4	C	502	YCD	C08-C06-N07-C09
4	C	502	YCD	C01-C06-N07-C09
3	A	502	Y8P	N07-C09-C17-C16
3	B	502	Y8P	N07-C09-C17-C16
4	C	502	YCD	N07-C09-C17-C16
3	B	502	Y8P	C01-C06-N07-C09
3	B	502	Y8P	C18-O40-P41-O42
3	A	502	Y8P	N07-C09-C17-C12
3	B	502	Y8P	N07-C09-C17-C12
4	C	502	YCD	N07-C09-C17-C12
3	B	502	Y8P	C01-C02-C03-O04
3	B	502	Y8P	C01-C02-C03-O05
3	B	502	Y8P	C18-O40-P41-O44
2	B	501	THR	O-C-CA-CB

There are no ring outliers.

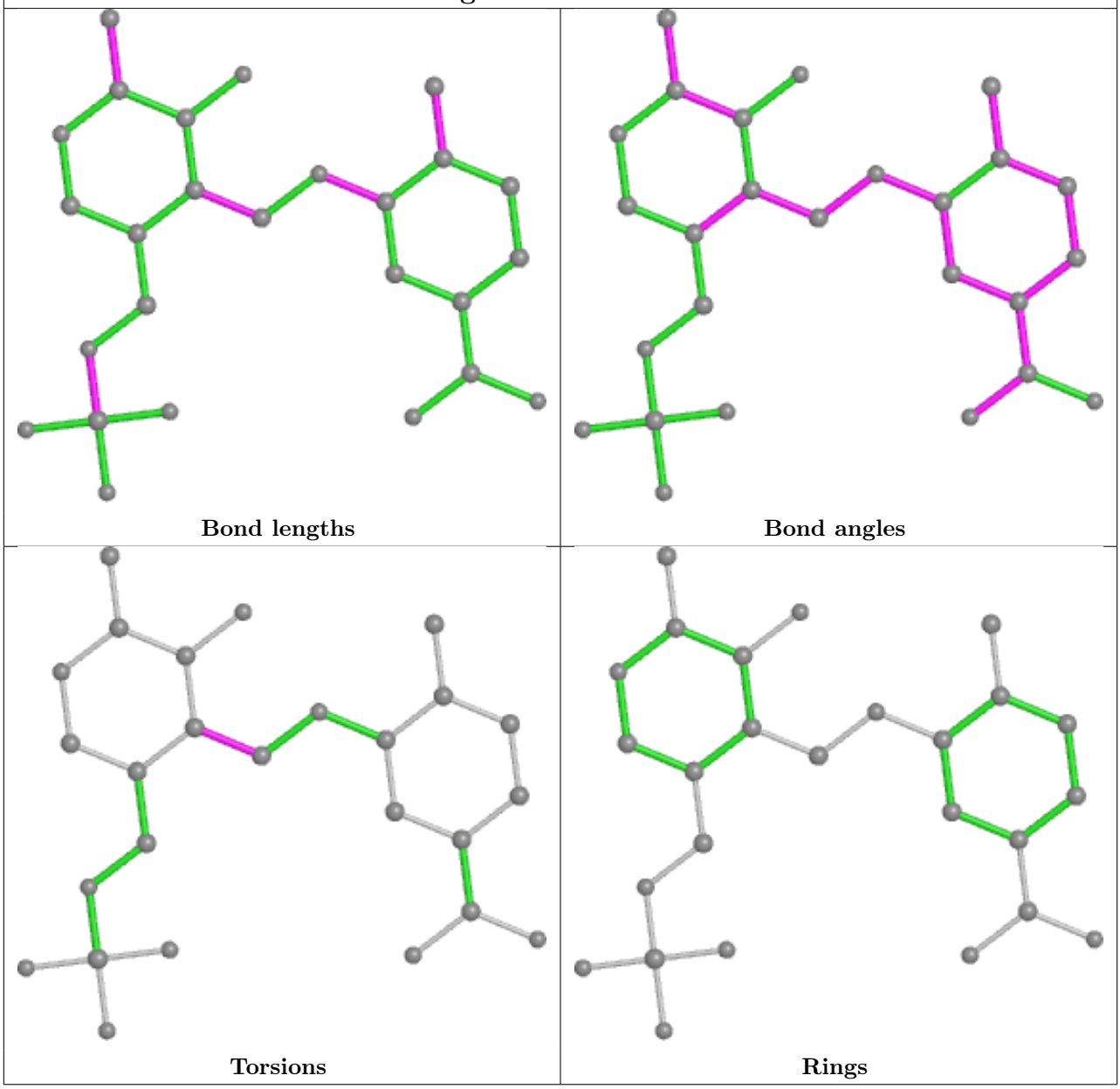
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	Y8P	1	0
2	C	501	THR	0	2
2	A	501	THR	0	2
4	C	502	YCD	2	0
3	B	502	Y8P	2	0

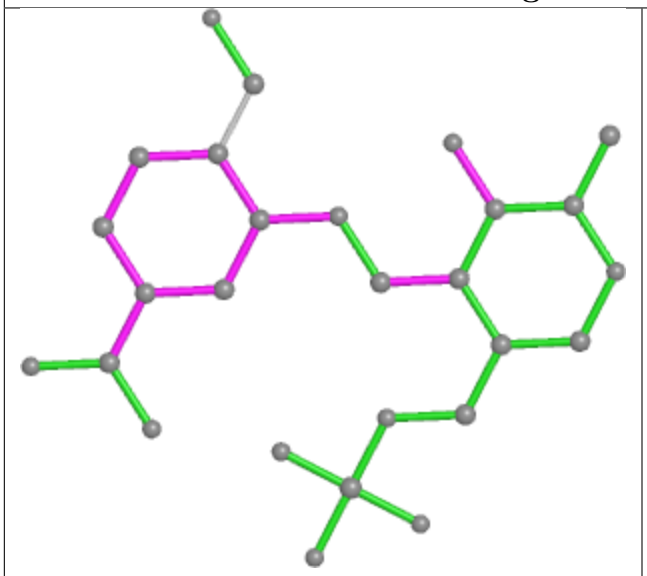
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

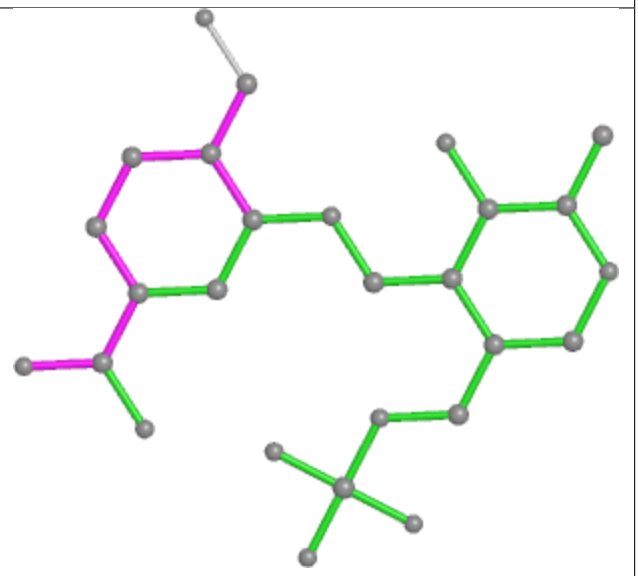
Ligand Y8P A 502



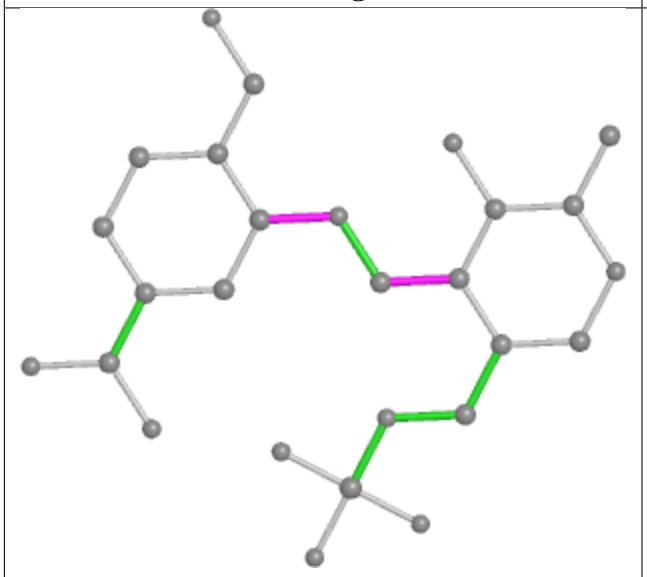
Ligand YCD C 502



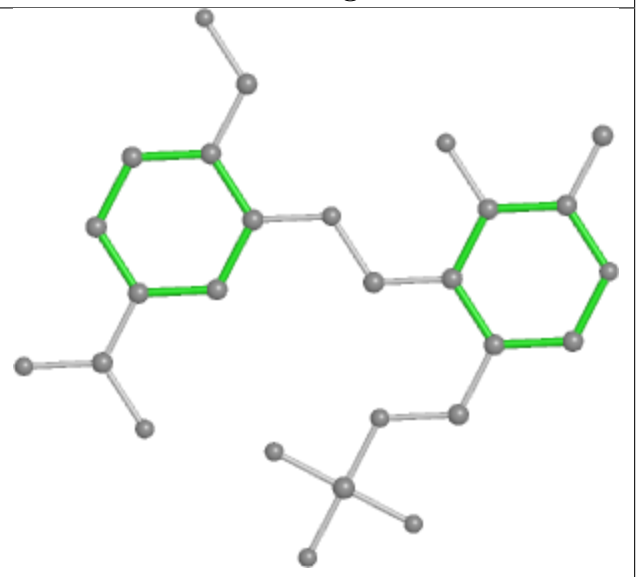
Bond lengths



Bond angles

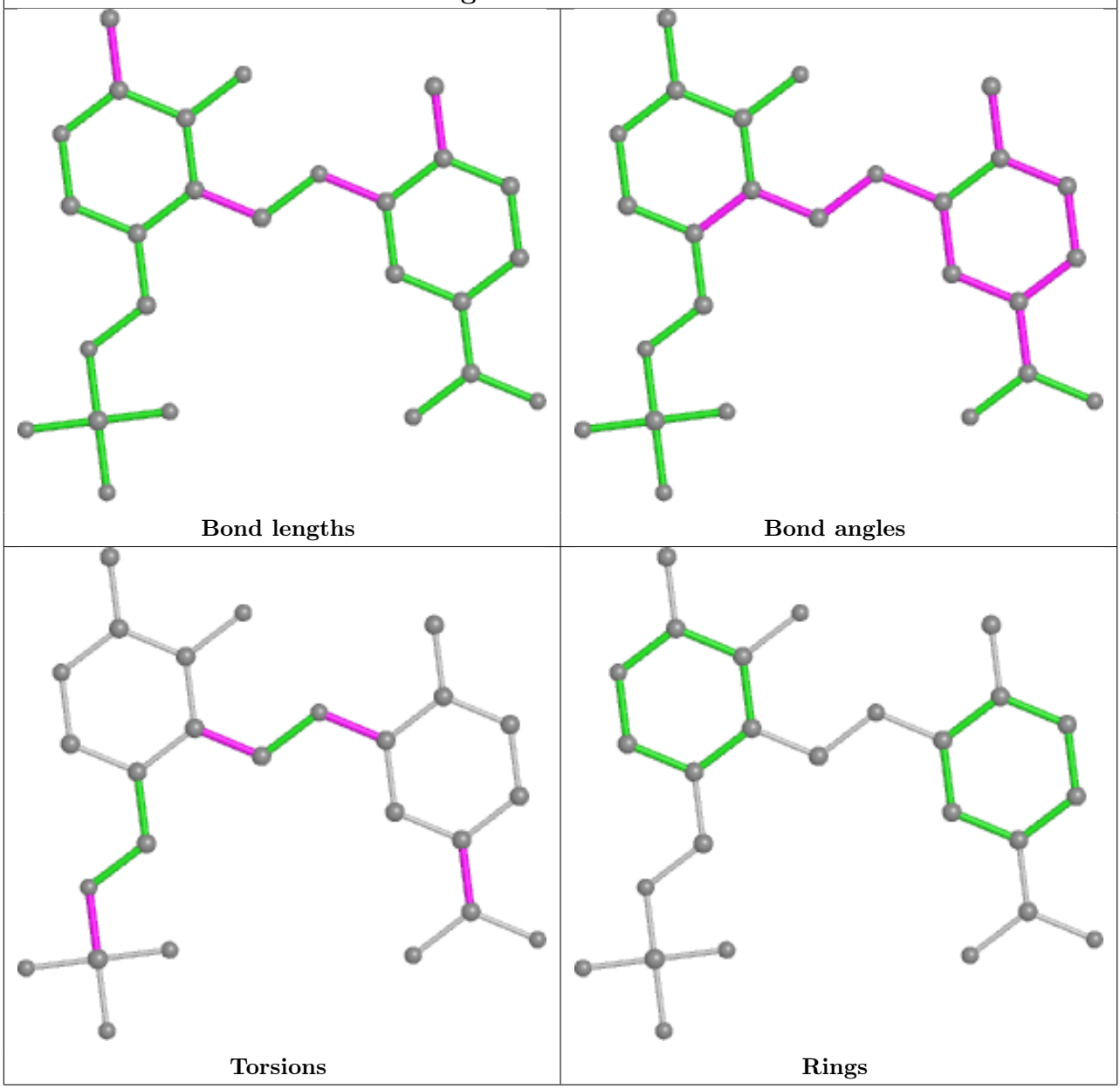


Torsions



Rings

Ligand Y8P B 502



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	402/404 (99%)	0.64	32 (7%) 12 16	32, 53, 79, 113	1 (0%)
1	B	402/404 (99%)	0.84	67 (16%) 1 2	34, 51, 88, 129	0
1	C	402/404 (99%)	0.52	37 (9%) 9 11	31, 44, 68, 120	0
All	All	1206/1212 (99%)	0.66	136 (11%) 5 6	31, 49, 81, 129	1 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	TRP	8.2
1	A	388	TRP	6.2
1	B	367	VAL	6.0
1	B	439	PHE	6.0
1	B	384	GLU	5.5
1	A	198	GLY	5.1
1	B	363	LEU	5.0
1	C	323	TYR	4.9
1	A	37	PRO	4.7
1	C	387	ASP	4.7
1	B	408	HIS	4.6
1	B	382	ILE	4.6
1	B	366	ASP	4.6
1	C	198	GLY	4.5
1	B	386	LYS	4.3
1	B	360	LEU	4.1
1	B	364	PRO	4.1
1	B	381	VAL	4.0
1	C	388	TRP	4.0
1	B	407	THR	3.9
1	B	383	LYS	3.9
1	B	141	THR	3.8
1	C	141	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	387	ASP	3.8
1	B	145	ALA	3.8
1	C	382	ILE	3.8
1	A	39	THR	3.8
1	A	386	LYS	3.7
1	C	179	GLY	3.7
1	B	265	ILE	3.6
1	A	387	ASP	3.6
1	B	392	LYS	3.6
1	A	367	VAL	3.6
1	B	355	ILE	3.5
1	C	386	LYS	3.5
1	B	198	GLY	3.4
1	A	143	VAL	3.3
1	A	408	HIS	3.2
1	A	141	THR	3.2
1	B	368	VAL	3.2
1	B	352	LEU	3.1
1	B	143	VAL	3.1
1	B	87	ALA	3.1
1	B	385	THR	3.1
1	B	321	SER	3.1
1	A	73	VAL	3.0
1	B	414	PHE	3.0
1	B	323	TYR	3.0
1	B	300	PRO	3.0
1	C	140	ASN	3.0
1	A	380	ILE	3.0
1	A	179	GLY	3.0
1	C	178	TRP	2.9
1	A	82	LEU	2.9
1	C	182	LEU	2.9
1	B	182	LEU	2.9
1	B	391	TRP	2.9
1	C	300	PRO	2.9
1	C	391	TRP	2.9
1	C	407	THR	2.9
1	B	365	SER	2.9
1	B	144	GLU	2.8
1	C	184	ALA	2.8
1	A	44	PHE	2.8
1	B	301	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	302	SER	2.8
1	B	184	ALA	2.7
1	A	301	VAL	2.7
1	A	383	LYS	2.7
1	B	421	LYS	2.7
1	C	439	PHE	2.7
1	B	437	LEU	2.7
1	A	142	GLY	2.7
1	C	385	THR	2.7
1	A	247	MET	2.7
1	B	324	GLY	2.6
1	C	37	PRO	2.6
1	A	410	ASP	2.6
1	C	185	ILE	2.6
1	C	321	SER	2.5
1	C	139	MET	2.5
1	C	436	ILE	2.5
1	A	71	TRP	2.5
1	B	369	THR	2.5
1	C	142	GLY	2.5
1	B	37	PRO	2.5
1	C	265	ILE	2.5
1	A	145	ALA	2.5
1	B	436	ILE	2.4
1	B	177	PHE	2.4
1	A	409	GLY	2.4
1	C	180	ARG	2.4
1	B	181	THR	2.4
1	B	291	GLY	2.4
1	C	177	PHE	2.3
1	C	45	GLU	2.3
1	C	304	VAL	2.3
1	B	86	SER	2.3
1	B	409	GLY	2.3
1	A	265	ILE	2.3
1	B	292	LYS	2.3
1	A	41	ASP	2.3
1	C	110	LEU	2.3
1	C	324	GLY	2.3
1	A	369	THR	2.3
1	B	142	GLY	2.3
1	B	289	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	166	TYR	2.2
1	C	299	TYR	2.2
1	B	347	GLU	2.2
1	B	179	GLY	2.2
1	A	99	ASN	2.2
1	C	302	SER	2.2
1	B	183	SER	2.2
1	C	143	VAL	2.2
1	A	292	LYS	2.2
1	C	146	GLY	2.2
1	B	320	GLY	2.2
1	C	366	ASP	2.1
1	B	297	GLY	2.1
1	A	185	ILE	2.1
1	B	43	ILE	2.1
1	B	434	LYS	2.1
1	A	50	TYR	2.1
1	B	295	SER	2.1
1	A	45	GLU	2.1
1	B	290	LEU	2.1
1	A	302	SER	2.1
1	B	71	TRP	2.1
1	B	81	PHE	2.1
1	B	178	TRP	2.1
1	C	325	GLY	2.1
1	B	298	LEU	2.1
1	B	84	SER	2.0
1	C	166	TYR	2.0
1	B	303	ALA	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)

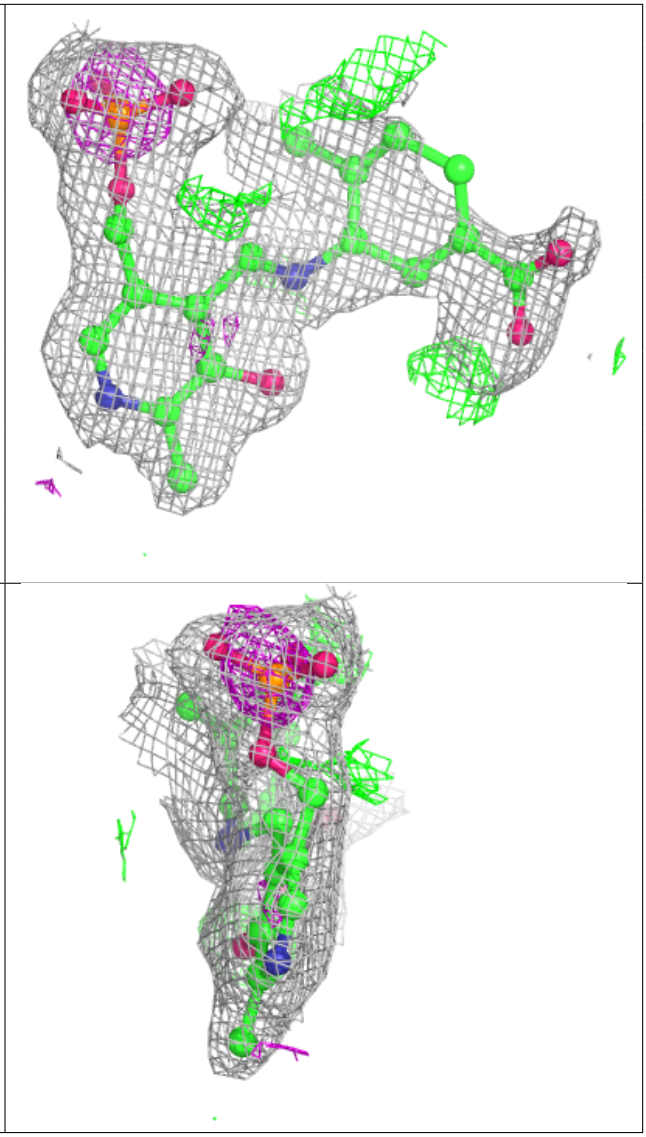
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

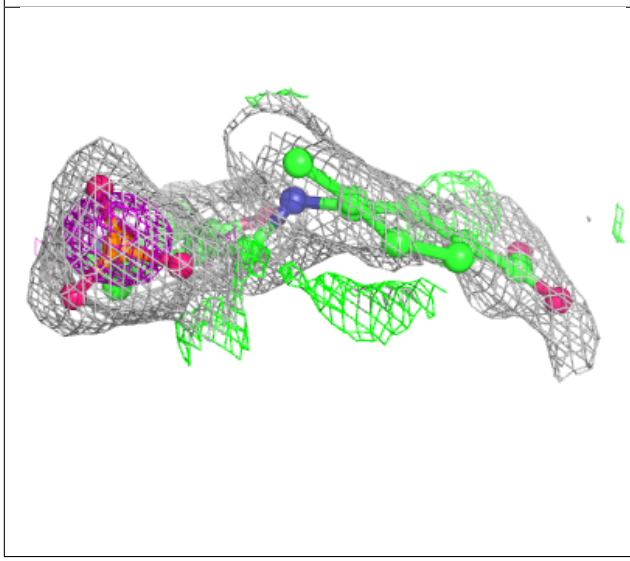
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	THR	C	501	7/8	0.84	0.31	46,48,50,51	1
3	Y8P	B	502	26/26	0.93	0.28	39,47,54,54	7
4	YCD	C	502	27/27	0.93	0.23	36,45,58,60	1
2	THR	B	501	7/8	0.94	0.36	41,43,48,48	1
3	Y8P	A	502	26/26	0.94	0.21	42,46,57,59	7
2	THR	A	501	7/8	0.95	0.22	44,45,49,49	1

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 Y8P B 502:

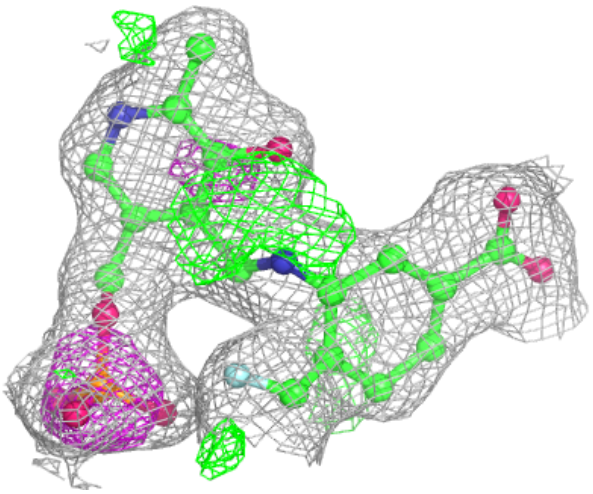
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

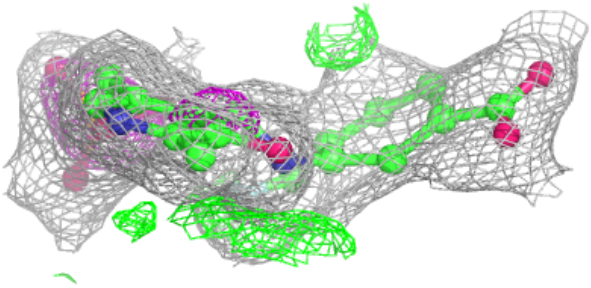


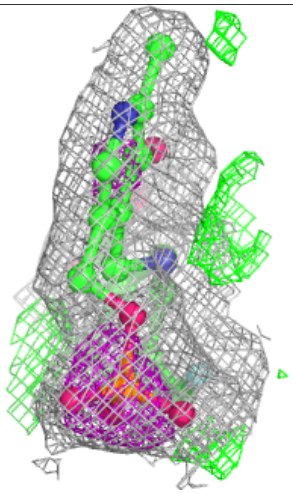


Electron density around YCD C 502:

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

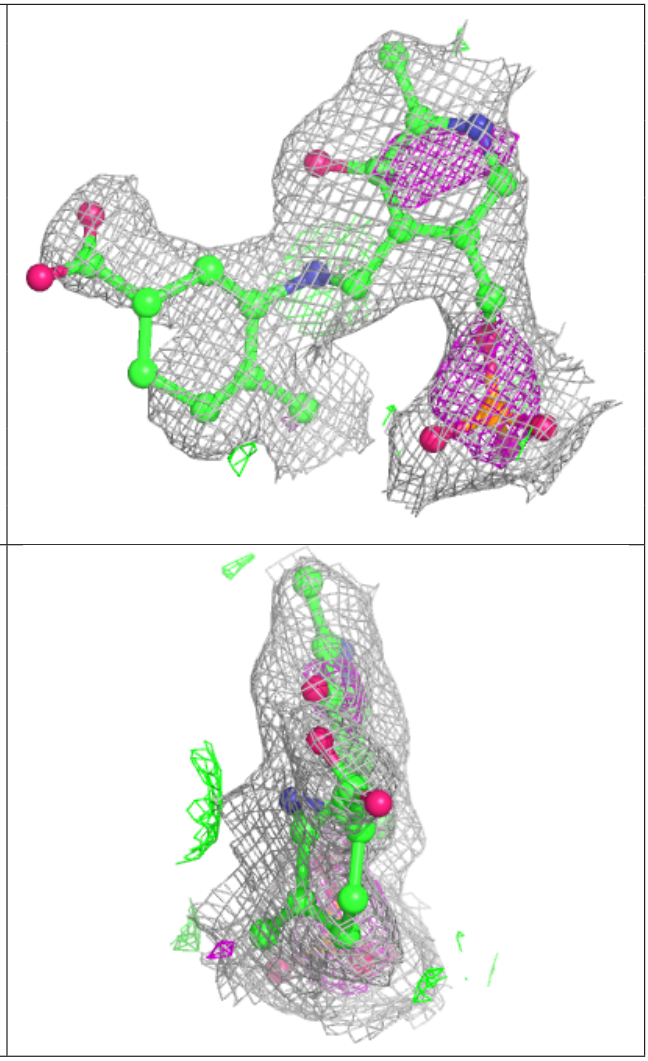






Electron density around Y8P A 502:

$2mF_o$-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.