



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:15 AM UTC

PDB ID : 4YU2 / pdb_00004yu2
Title : Crystal structure of DYRK1A with harmine-derivatized AnnH-75 inhibitor
Authors : Chaikuad, A.; Wurzlbauer, A.; Nowak, R.; von Delft, F.; Arrowsmith, C.H.;
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Consortium (SGC)
Deposited on : 2015-03-18
Resolution : 2.90 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

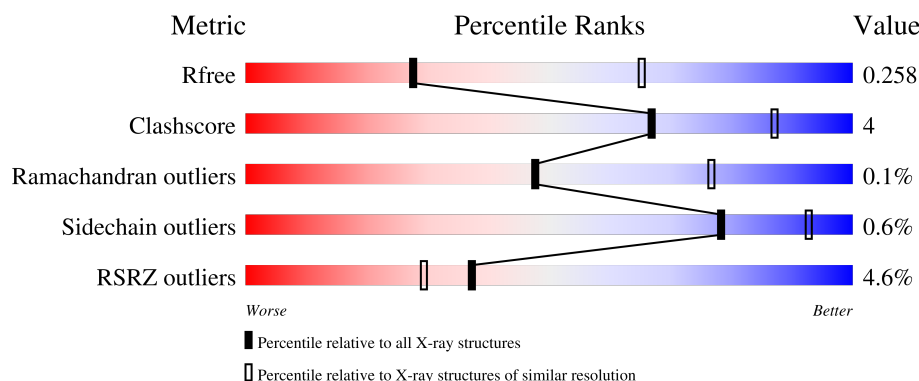
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	361	2% 88% 8% ..
1	B	361	3% 87% 9% .
1	C	361	6% 89% 7% .
1	D	361	6% 89% 7% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11762 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.

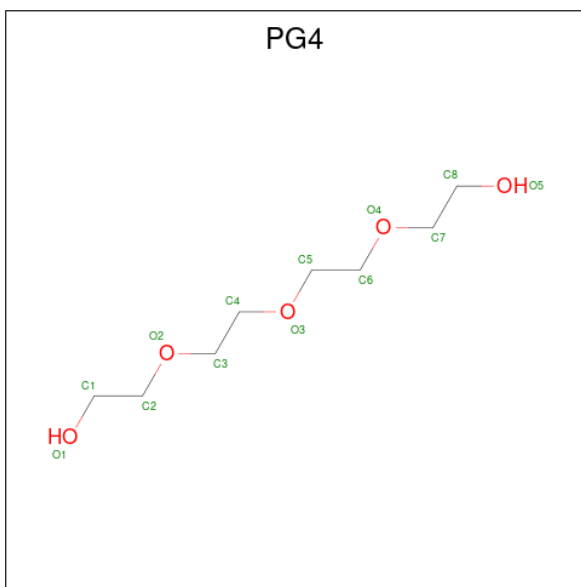
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	P	S	0	1	0
			2846	1827	486	514	2	17			
1	B	348	Total	C	N	O	P	S	0	1	0
			2821	1810	479	513	2	17			
1	C	347	Total	C	N	O	P	S	0	2	0
			2828	1816	485	508	2	17			
1	D	347	Total	C	N	O	P	S	0	2	0
			2826	1813	483	512	2	16			

There are 8 discrepancies between the modelled and reference sequences:

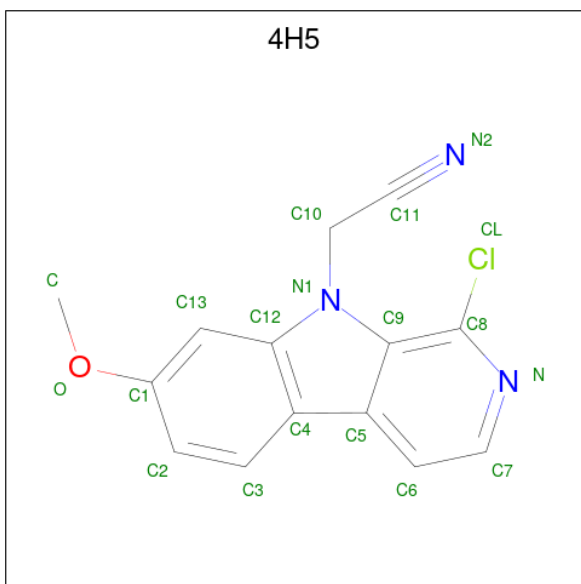
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627
D	126	MET	-	expression tag	UNP Q13627

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is (1-chloro-7-methoxy-9H-beta-carboline-9-yl)acetonitrile (CCD ID: 4H5) (formula: $C_{14}H_{10}ClN_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			19	14	1	3	1		
3	B	1	Total	C	Cl	N	O	0	0
			19	14	1	3	1		
3	C	1	Total	C	Cl	N	O	0	0
			19	14	1	3	1		
3	D	1	Total	C	Cl	N	O	0	0
			19	14	1	3	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	90	Total	O	0	0
			90	90		

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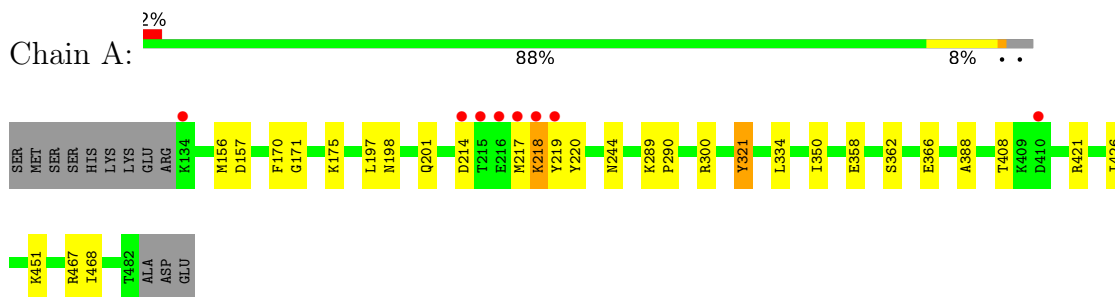
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	54	Total	O	0	0
			54	54		
5	D	54	Total	O	0	0
			54	54		

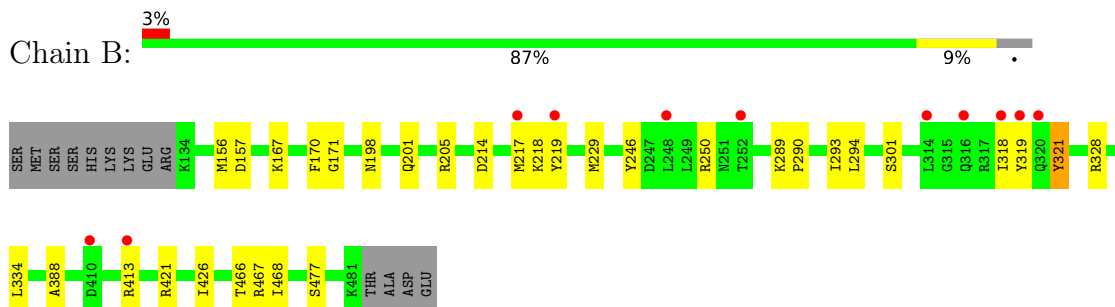
3 Residue-property plots [i](#)

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.

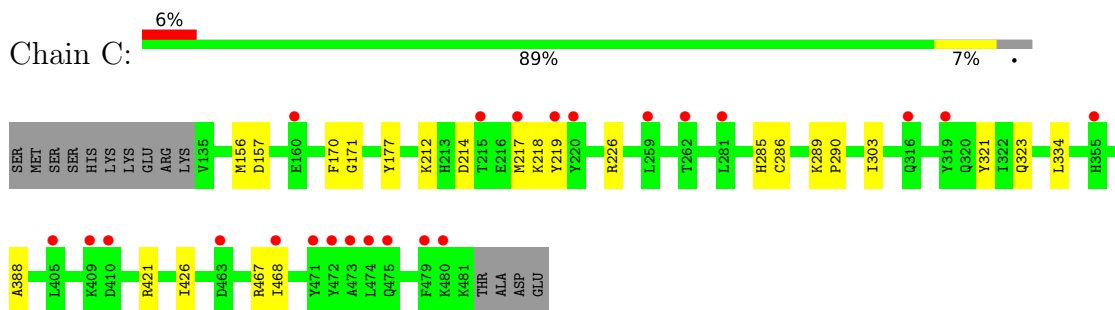
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



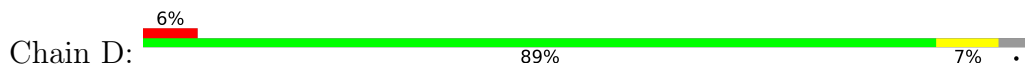
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

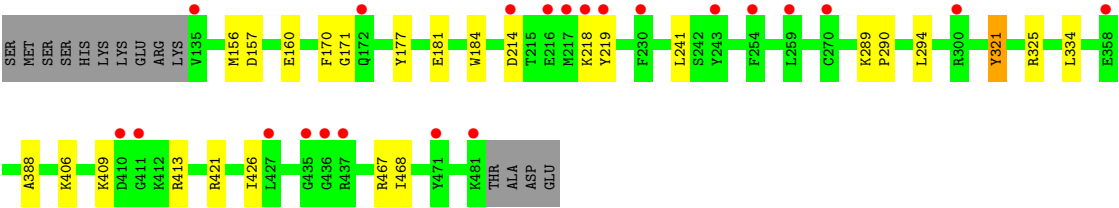


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	265.57Å 65.44Å 138.65Å 90.00° 114.44° 90.00°	Depositor
Resolution (Å)	48.34 – 2.90 48.34 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.34-2.90) 99.3 (48.34-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.243 , 0.277 (Not available) , 0.258	Depositor DCC
R_{free} test set	2443 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11762	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.45% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, 4H5, PG4, SO4

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	0.81	0/2882	0.80	0/3889
1	B	0.75	0/2857	0.76	0/3861
1	C	0.71	0/2867	0.76	1/3869 (0.0%)
1	D	0.69	1/2865 (0.0%)	0.75	0/3869
All	All	0.74	1/11471 (0.0%)	0.77	1/15488 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	413	ARG	CA-C	-6.02	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	ILE	N-CA-C	5.02	117.23	108.95

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	LYS	Peptide
1	A	408	THR	Peptide
1	B	218	LYS	Peptide
1	C	218	LYS	Peptide
1	D	218	LYS	Peptide
1	D	409	LYS	Peptide

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	2846	0	2815	24	0
1	B	2821	0	2759	25	0
1	C	2828	0	2791	15	0
1	D	2826	0	2776	22	0
2	A	13	0	18	1	0
2	B	13	0	18	3	0
2	C	13	0	18	0	0
3	A	19	0	10	2	0
3	B	19	0	10	4	0
3	C	19	0	10	1	0
3	D	19	0	10	3	0
4	B	15	0	0	1	0
4	C	5	0	0	0	0
5	A	108	0	0	7	0
5	B	90	0	0	3	0
5	C	54	0	0	2	0
5	D	54	0	0	1	0
All	All	11762	0	11235	83	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 (83) 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:250:ARG:NH1	1:D:160:GLU:OE2	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:LYS:CD	1:D:181:GLU:OE1	2.33	0.77
1:B:229:MET:HE3	2:B:501:PG4:H41	1.68	0.74
3:A:502:4H5:H3	3:A:502:4H5:CL	2.28	0.71
1:D:321[B]:PTR:O1P	1:D:321[B]:PTR:HE2	1.91	0.70
1:A:214:ASP:OD2	5:A:673:HOH:O	2.11	0.68
1:B:167:LYS:HD3	1:D:181:GLU:OE1	1.94	0.68
1:B:250:ARG:NH1	1:D:177:TYR:CD2	2.62	0.67
1:A:300:ARG:HD3	1:C:177:TYR:CZ	2.30	0.65
1:D:406:LYS:HE2	5:D:654:HOH:O	1.97	0.65
1:B:167:LYS:HD2	1:D:181:GLU:OE1	1.95	0.65
1:A:321[B]:PTR:O3P	1:A:366:GLU:HG3	1.98	0.63
1:A:300:ARG:HD3	1:C:177:TYR:CE1	2.35	0.62
1:B:321[B]:PTR:O3P	1:B:328:ARG:NH2	2.23	0.62
3:A:502:4H5:CL	3:A:502:4H5:C10	2.85	0.61
3:C:502:4H5:H3	3:C:502:4H5:CL	2.38	0.60
1:A:451:LYS:HE2	5:A:701:HOH:O	2.05	0.57
1:A:175:LYS:NZ	5:A:664:HOH:O	2.38	0.57
1:A:300:ARG:CD	1:C:177:TYR:CZ	2.88	0.56
3:B:502:4H5:CL	3:B:502:4H5:H3	2.45	0.53
1:B:318:ILE:HG23	1:B:319:TYR:CD2	2.43	0.53
1:A:321[B]:PTR:P	5:A:624:HOH:O	2.67	0.52
1:B:246:TYR:HH	1:D:184:TRP:HZ2	1.53	0.52
3:B:502:4H5:C11	3:B:502:4H5:H5	2.39	0.51
1:A:170:PHE:CD1	1:A:171:GLY:N	2.78	0.51
3:B:502:4H5:H4	5:B:618:HOH:O	2.11	0.50
1:A:289:LYS:O	1:A:290:PRO:C	2.55	0.50
1:A:300:ARG:CD	1:C:177:TYR:CE1	2.95	0.49
1:A:334:LEU:HB3	1:A:388:ALA:HB1	1.95	0.49
1:D:294:LEU:HD23	3:D:501:4H5:H8	1.95	0.49
1:B:334:LEU:HB3	1:B:388:ALA:HB1	1.95	0.48
1:D:334:LEU:HB3	1:D:388:ALA:HB1	1.95	0.48
1:A:214:ASP:CG	1:A:219:TYR:HB2	2.38	0.48
1:C:334:LEU:HB3	1:C:388:ALA:HB1	1.96	0.48
1:B:301:SER:OG	4:B:504:SO4:O4	2.29	0.47
1:D:170:PHE:CD1	1:D:171:GLY:N	2.82	0.47
1:D:214:ASP:CG	1:D:219:TYR:HB2	2.39	0.47
1:B:201:GLN:OE1	2:B:501:PG4:H61	2.15	0.47
1:C:170:PHE:CD1	1:C:171:GLY:N	2.83	0.46
1:C:214:ASP:CG	1:C:219:TYR:HB2	2.40	0.46
1:A:197:LEU:HD21	2:A:501:PG4:H52	1.98	0.46
3:D:501:4H5:H3	3:D:501:4H5:CL	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASN:HA	1:A:201:GLN:HE21	1.80	0.45
1:B:214:ASP:CG	1:B:219:TYR:HB2	2.41	0.45
3:B:502:4H5:C11	3:B:502:4H5:C13	2.94	0.45
1:B:289:LYS:O	1:B:290:PRO:C	2.60	0.45
1:B:246:TYR:OH	1:D:184:TRP:HZ2	2.00	0.45
1:B:467:ARG:O	1:B:468:ILE:C	2.60	0.44
1:C:214:ASP:OD2	1:C:219:TYR:HB2	2.17	0.44
1:B:170:PHE:CD1	1:B:171:GLY:N	2.85	0.44
1:D:467:ARG:O	1:D:468:ILE:C	2.60	0.44
1:A:467:ARG:O	1:A:468:ILE:C	2.61	0.44
1:D:214:ASP:OD2	1:D:219:TYR:HB2	2.18	0.44
1:C:289:LYS:O	1:C:290:PRO:C	2.60	0.43
1:B:156:MET:O	1:B:157:ASP:C	2.61	0.43
1:A:214:ASP:OD2	1:A:219:TYR:HB2	2.17	0.43
1:B:293:ILE:C	1:B:294:LEU:HD12	2.43	0.43
1:C:467:ARG:O	1:C:468:ILE:C	2.61	0.43
1:D:289:LYS:O	1:D:290:PRO:C	2.60	0.43
1:B:214:ASP:OD2	1:B:219:TYR:HB2	2.18	0.42
1:C:156:MET:O	1:C:157:ASP:C	2.62	0.42
1:D:241:LEU:O	3:D:501:4H5:H6	2.19	0.42
1:D:156:MET:O	1:D:157:ASP:C	2.62	0.42
1:A:219:TYR:O	1:A:220:TYR:HB2	2.19	0.42
1:D:321[B]:PTR:O1P	1:D:321[B]:PTR:CE2	2.66	0.42
1:B:198:ASN:HA	1:B:201:GLN:HE21	1.85	0.42
1:A:244:ASN:ND2	5:A:640:HOH:O	2.53	0.42
1:D:321[A]:PTR:O2P	1:D:325:ARG:NH1	2.53	0.41
1:D:421:ARG:HG2	1:D:426:ILE:HD11	2.01	0.41
1:D:321[A]:PTR:O3P	1:D:321[A]:PTR:HE1	2.20	0.41
1:B:201:GLN:HG2	2:B:501:PG4:H12	2.02	0.41
1:B:421:ARG:HG2	1:B:426:ILE:HD11	2.01	0.41
1:C:212:LYS:HD3	5:C:612:HOH:O	2.20	0.41
1:A:321[A]:PTR:O3P	5:A:601:HOH:O	2.22	0.41
1:B:205:ARG:HG3	5:B:690:HOH:O	2.21	0.41
1:A:358:GLU:HG3	5:A:697:HOH:O	2.21	0.41
1:C:226[A]:ARG:HD3	5:C:624:HOH:O	2.21	0.41
1:C:285:HIS:O	1:C:286:CYS:HB2	2.21	0.41
1:B:413:ARG:N	5:B:610:HOH:O	2.52	0.41
1:A:290:PRO:HD3	1:A:350:ILE:HG12	2.03	0.40
1:A:156:MET:O	1:A:157:ASP:C	2.64	0.40
1:C:421:ARG:HG2	1:C:426:ILE:HD11	2.03	0.40
1:A:421:ARG:HG2	1:A:426:ILE:HD11	2.03	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	346/361 (96%)	320 (92%)	26 (8%)	0	100	100
1	B	345/361 (96%)	322 (93%)	23 (7%)	0	100	100
1	C	345/361 (96%)	320 (93%)	24 (7%)	1 (0%)	36	65
1	D	345/361 (96%)	319 (92%)	26 (8%)	0	100	100
All	All	1381/1444 (96%)	1281 (93%)	99 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	323	GLN

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	302/320 (94%)	299 (99%)	3 (1%)	68	89
1	B	297/320 (93%)	294 (99%)	3 (1%)	68	89
1	C	298/320 (93%)	297 (100%)	1 (0%)	86	96
1	D	298/320 (93%)	298 (100%)	0	100	100
All	All	1195/1280 (93%)	1188 (99%)	7 (1%)	78	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	MET
1	A	218	LYS
1	A	362	SER
1	B	217	MET
1	B	466	THR
1	B	477	SER
1	C	217	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	198	ASN
1	A	232	ASN
1	B	172	GLN
1	B	232	ASN
1	B	424	HIS
1	C	172	GLN
1	C	232	ASN
1	C	383	HIS
1	D	172	GLN
1	D	232	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	PTR	B	321[B]	-	15,16,17	0.77	0	17,22,24	1.04	1 (5%)
1	PTR	D	321[A]	-	15,16,17	0.89	0	17,22,24	0.98	1 (5%)
1	PTR	C	321[B]	-	15,16,17	1.03	0	17,22,24	1.13	2 (11%)
1	PTR	A	321[B]	-	15,16,17	0.79	0	17,22,24	0.82	0
1	PTR	B	321[A]	-	15,16,17	1.39	2 (13%)	17,22,24	1.03	1 (5%)
1	PTR	D	321[B]	-	15,16,17	0.97	0	17,22,24	1.02	0
1	PTR	C	321[A]	-	15,16,17	0.90	0	17,22,24	1.15	1 (5%)
1	PTR	A	321[A]	-	15,16,17	0.89	0	17,22,24	1.10	1 (5%)

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
1	PTR	B	321[B]	-	-	1/10/11/13	0/1/1/1
1	PTR	D	321[A]	-	-	1/10/11/13	0/1/1/1
1	PTR	C	321[B]	-	-	3/10/11/13	0/1/1/1
1	PTR	A	321[B]	-	-	3/10/11/13	0/1/1/1
1	PTR	B	321[A]	-	-	3/10/11/13	0/1/1/1
1	PTR	D	321[B]	-	-	3/10/11/13	0/1/1/1
1	PTR	C	321[A]	-	-	1/10/11/13	0/1/1/1
1	PTR	A	321[A]	-	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321[A]	PTR	CB-CA	3.39	1.60	1.53
1	B	321[A]	PTR	P-OH	2.23	1.63	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321[A]	PTR	O3P-P-O2P	2.98	118.96	107.80
1	D	321[A]	PTR	O3P-P-O2P	2.43	116.90	107.80
1	B	321[A]	PTR	P-OH-CZ	2.40	132.43	123.88
1	C	321[B]	PTR	CB-CG-CD1	-2.33	116.56	120.90
1	C	321[B]	PTR	CB-CG-CD2	2.32	125.21	120.90
1	B	321[B]	PTR	O2P-P-O1P	2.06	118.86	110.83
1	A	321[A]	PTR	O2P-P-OH	-2.02	99.36	105.32

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	321[A]	PTR	O-C-CA-CB
1	A	321[B]	PTR	O-C-CA-CB
1	A	321[B]	PTR	CZ-OH-P-O1P
1	B	321[A]	PTR	O-C-CA-CB
1	B	321[A]	PTR	N-CA-CB-CG
1	B	321[A]	PTR	C-CA-CB-CG
1	B	321[B]	PTR	O-C-CA-CB
1	C	321[A]	PTR	O-C-CA-CB
1	C	321[B]	PTR	O-C-CA-CB
1	C	321[B]	PTR	N-CA-CB-CG
1	C	321[B]	PTR	C-CA-CB-CG
1	D	321[A]	PTR	O-C-CA-CB
1	D	321[B]	PTR	O-C-CA-CB
1	D	321[B]	PTR	N-CA-CB-CG
1	D	321[B]	PTR	C-CA-CB-CG
1	A	321[B]	PTR	CZ-OH-P-O3P

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321[B]	PTR	1	0
1	D	321[A]	PTR	2	0
1	A	321[B]	PTR	2	0
1	D	321[B]	PTR	2	0
1	A	321[A]	PTR	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 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	4H5	A	502	-	21,21,21	2.01	4 (19%)	28,30,30	2.59	10 (35%)
2	PG4	B	501	-	12,12,12	0.74	0	11,11,11	0.68	0
3	4H5	D	501	-	21,21,21	1.48	3 (14%)	28,30,30	2.09	7 (25%)
4	SO4	B	503	-	4,4,4	0.46	0	6,6,6	0.26	0
2	PG4	C	501	-	12,12,12	0.62	0	11,11,11	0.28	0
3	4H5	C	502	-	21,21,21	1.37	2 (9%)	28,30,30	1.96	5 (17%)
4	SO4	B	505	-	4,4,4	0.60	0	6,6,6	0.23	0
4	SO4	B	504	-	4,4,4	0.50	0	6,6,6	0.21	0
2	PG4	A	501	-	12,12,12	0.63	0	11,11,11	0.68	0
4	SO4	C	503	-	4,4,4	0.54	0	6,6,6	0.41	0
3	4H5	B	502	-	21,21,21	1.73	4 (19%)	28,30,30	2.08	7 (25%)

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	4H5	A	502	-	-	2/4/5/5	0/3/3/3
2	PG4	B	501	-	-	8/10/10/10	-
3	4H5	D	501	-	-	2/4/5/5	0/3/3/3
2	PG4	C	501	-	-	6/10/10/10	-
3	4H5	C	502	-	-	4/4/5/5	0/3/3/3
2	PG4	A	501	-	-	4/10/10/10	-
3	4H5	B	502	-	-	4/4/5/5	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	4H5	C5-C9	-6.12	1.32	1.41
3	D	501	4H5	C5-C9	-4.49	1.34	1.41
3	C	502	4H5	C5-C9	-4.33	1.34	1.41
3	B	502	4H5	C8-CL	3.99	1.81	1.74
3	A	502	4H5	C4-C12	-3.94	1.35	1.41
3	B	502	4H5	C5-C9	-3.93	1.35	1.41
3	B	502	4H5	C8-N	3.73	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	4H5	C4-C12	-2.70	1.37	1.41
3	D	501	4H5	C4-C12	-2.64	1.37	1.41
3	A	502	4H5	C9-N1	-2.61	1.36	1.40
3	B	502	4H5	C4-C12	-2.46	1.37	1.41
3	D	501	4H5	C8-CL	2.36	1.78	1.74
3	A	502	4H5	C3-C4	-2.29	1.36	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	4H5	C13-C12-N1	6.14	136.76	128.53
3	A	502	4H5	C10-C11-N2	-5.70	170.00	177.91
3	B	502	4H5	C7-N-C8	5.66	121.41	116.80
3	D	501	4H5	C7-N-C8	5.33	121.14	116.80
3	C	502	4H5	C7-N-C8	5.20	121.03	116.80
3	D	501	4H5	C13-C12-N1	4.88	135.07	128.53
3	A	502	4H5	C3-C4-C12	4.74	124.71	119.24
3	A	502	4H5	C13-C12-C4	-4.42	116.95	122.04
3	A	502	4H5	C7-N-C8	4.36	120.35	116.80
3	B	502	4H5	C10-C11-N2	-4.32	171.91	177.91
3	C	502	4H5	C13-C12-N1	4.32	134.32	128.53
3	B	502	4H5	C13-C12-N1	3.93	133.79	128.53
3	C	502	4H5	C3-C4-C12	3.70	123.51	119.24
3	D	501	4H5	C3-C4-C12	3.70	123.51	119.24
3	A	502	4H5	C10-N1-C12	3.57	129.45	124.94
3	D	501	4H5	C13-C12-C4	-3.41	118.12	122.04
3	B	502	4H5	C3-C4-C12	3.38	123.14	119.24
3	D	501	4H5	C-O-C1	3.32	124.62	117.50
3	A	502	4H5	C6-C7-N	-3.26	119.98	123.97
3	C	502	4H5	C13-C12-C4	-3.01	118.58	122.04
3	D	501	4H5	C6-C7-N	-2.88	120.44	123.97
3	B	502	4H5	C6-C7-N	-2.78	120.56	123.97
3	A	502	4H5	C4-C12-N1	-2.74	106.28	109.20
3	C	502	4H5	C6-C7-N	-2.60	120.78	123.97
3	B	502	4H5	C13-C12-C4	-2.57	119.09	122.04
3	D	501	4H5	C4-C12-N1	-2.26	106.80	109.20
3	A	502	4H5	C-O-C1	2.24	122.30	117.50
3	A	502	4H5	CL-C8-N	2.05	119.09	115.98
3	B	502	4H5	C9-C8-N	-2.01	119.00	122.04

There are no chirality outliers.

All (30) torsion outliers are listed below:

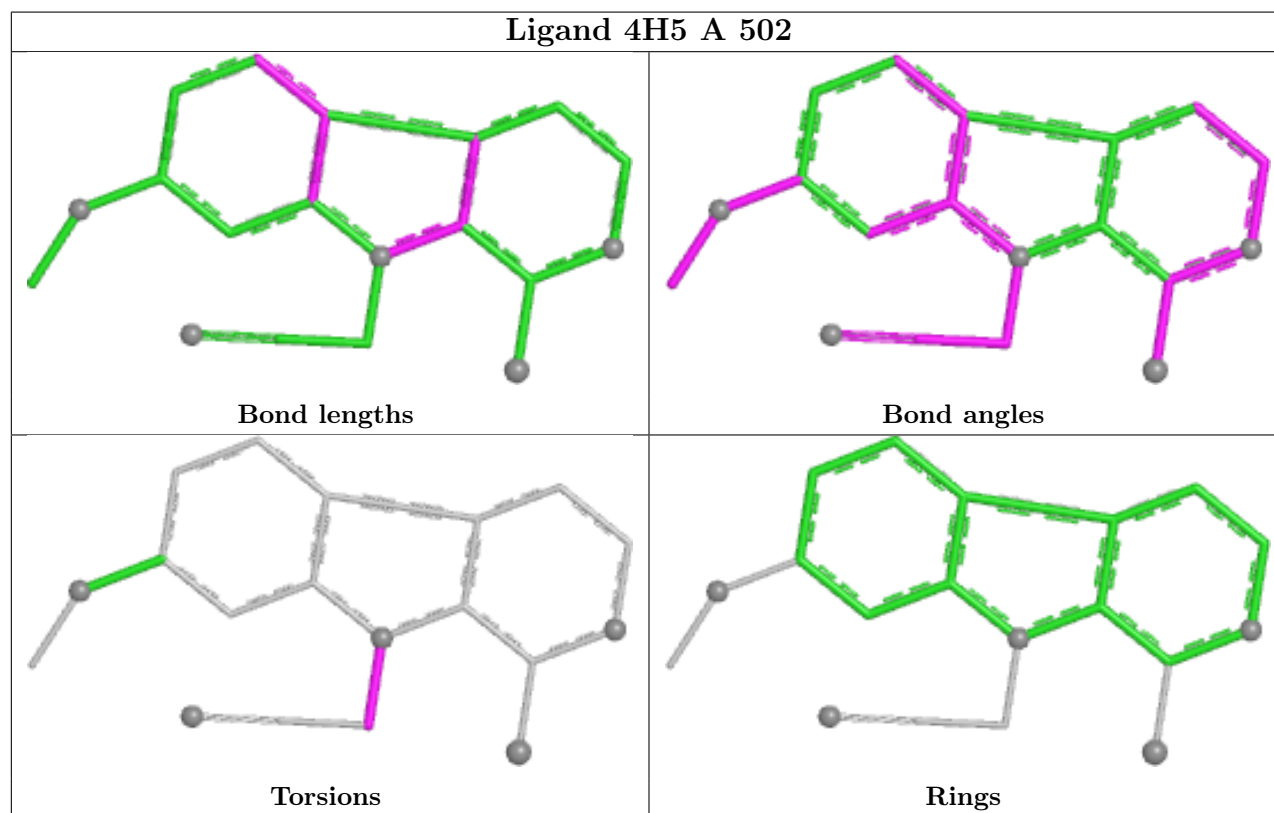
Mol	Chain	Res	Type	Atoms
3	A	502	4H5	C11-C10-N1-C9
3	A	502	4H5	C11-C10-N1-C12
3	B	502	4H5	C11-C10-N1-C9
3	B	502	4H5	C11-C10-N1-C12
3	C	502	4H5	C11-C10-N1-C9
2	B	501	PG4	C8-C7-O4-C6
2	A	501	PG4	O2-C3-C4-O3
2	A	501	PG4	O3-C5-C6-O4
2	C	501	PG4	O2-C3-C4-O3
2	C	501	PG4	O1-C1-C2-O2
2	B	501	PG4	O2-C3-C4-O3
2	A	501	PG4	O4-C7-C8-O5
3	C	502	4H5	C13-C1-O-C
3	C	502	4H5	C2-C1-O-C
2	B	501	PG4	O1-C1-C2-O2
2	C	501	PG4	C8-C7-O4-C6
2	B	501	PG4	C6-C5-O3-C4
3	B	502	4H5	C13-C1-O-C
3	B	502	4H5	C2-C1-O-C
2	A	501	PG4	C6-C5-O3-C4
2	C	501	PG4	C4-C3-O2-C2
2	B	501	PG4	O4-C7-C8-O5
2	B	501	PG4	C1-C2-O2-C3
3	D	501	4H5	C13-C1-O-C
3	C	502	4H5	C11-C10-N1-C12
3	D	501	4H5	C2-C1-O-C
2	C	501	PG4	C3-C4-O3-C5
2	B	501	PG4	C3-C4-O3-C5
2	B	501	PG4	O3-C5-C6-O4
2	C	501	PG4	C6-C5-O3-C4

There are no ring outliers.

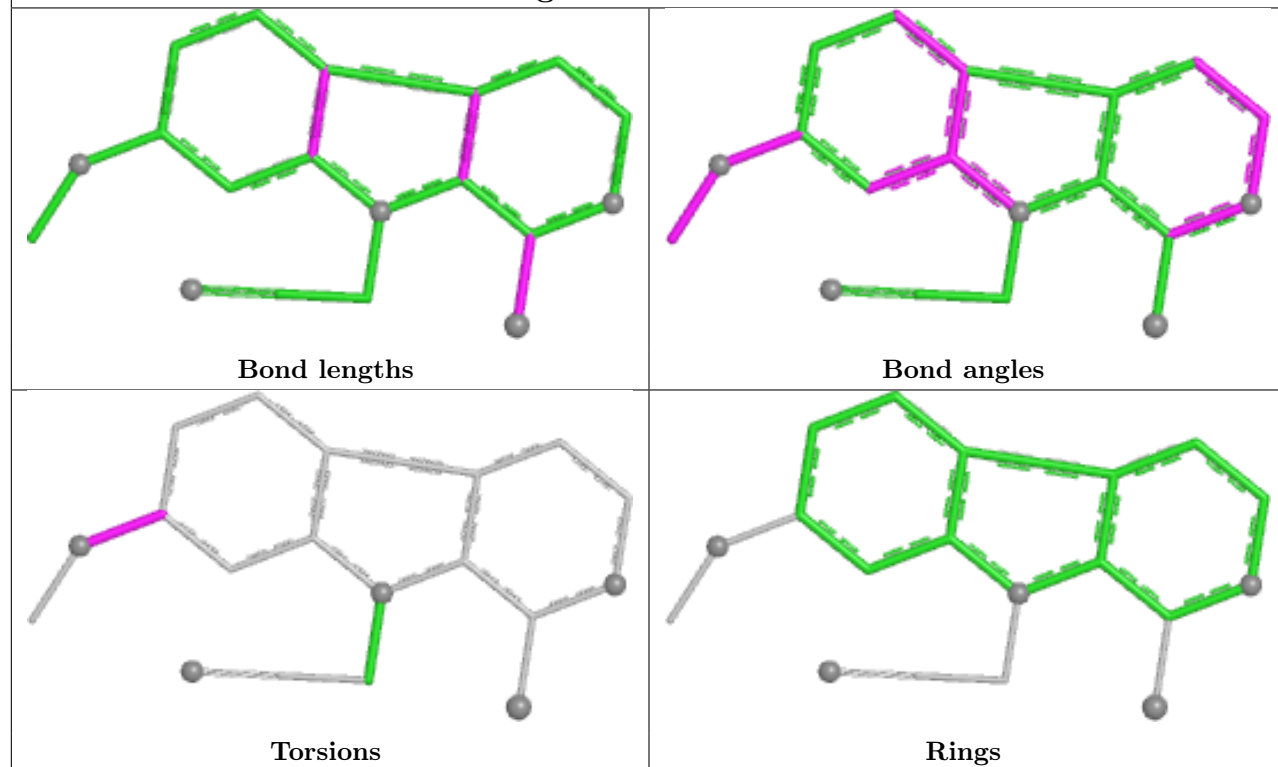
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	4H5	2	0
2	B	501	PG4	3	0
3	D	501	4H5	3	0
3	C	502	4H5	1	0
4	B	504	SO4	1	0
2	A	501	PG4	1	0
3	B	502	4H5	4	0

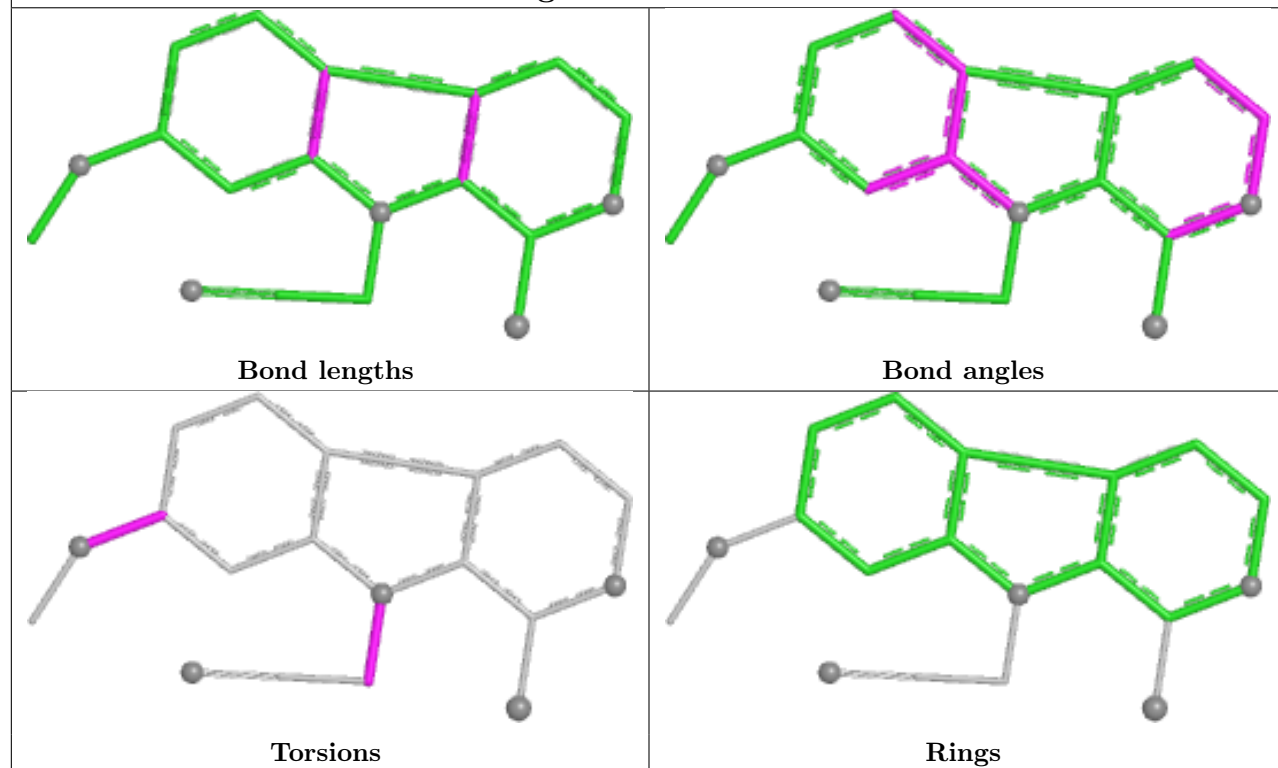
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

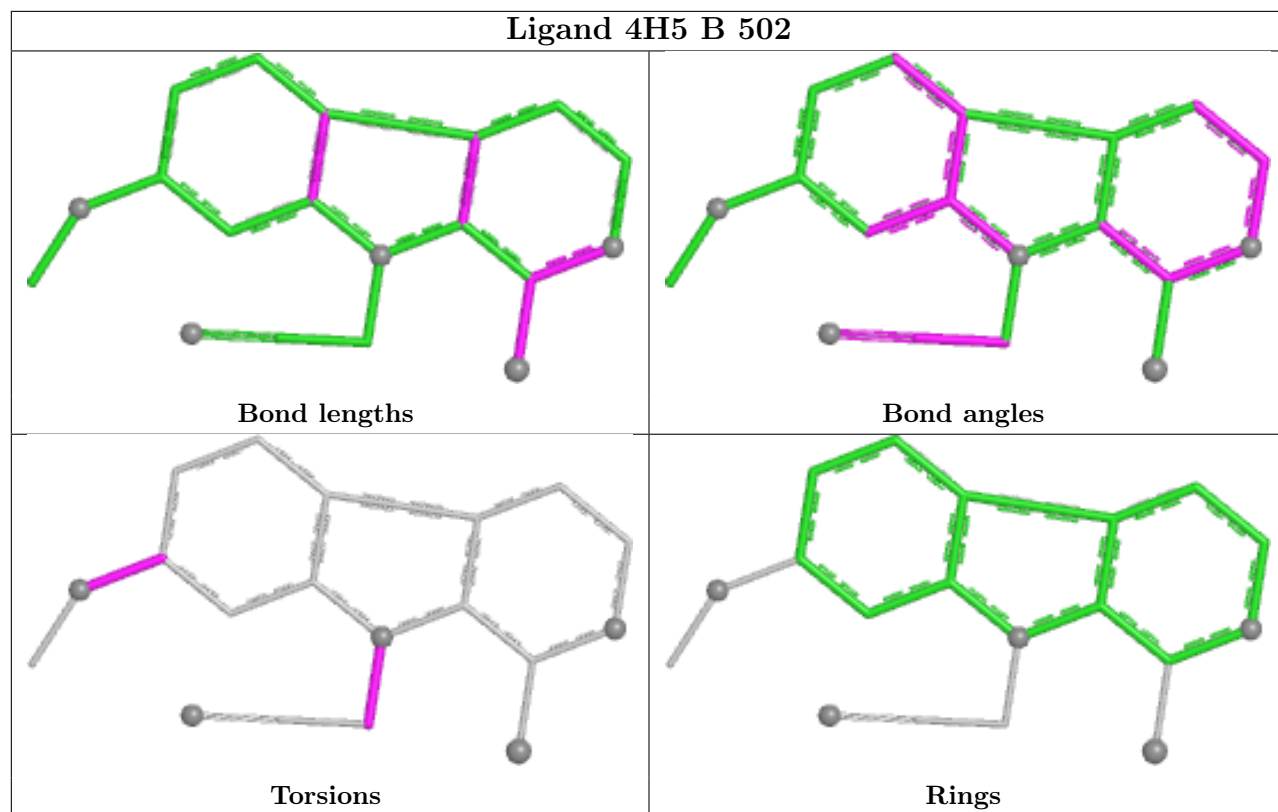


Ligand 4H5 D 501



Ligand 4H5 C 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

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, 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	348/361 (96%)	0.23	8 (2%) 61 52	30, 54, 94, 174	0
1	B	347/361 (96%)	0.51	11 (3%) 50 41	44, 71, 115, 174	0
1	C	346/361 (95%)	0.69	23 (6%) 24 19	44, 80, 114, 137	1 (0%)
1	D	346/361 (95%)	0.71	22 (6%) 25 20	51, 82, 122, 148	1 (0%)
All	All	1387/1444 (96%)	0.53	64 (4%) 37 29	30, 73, 116, 174	2 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	MET	5.9
1	A	219	TYR	4.9
1	B	318	ILE	4.8
1	D	217	MET	4.6
1	A	218	LYS	4.3
1	C	474	LEU	3.7
1	B	319	TYR	3.7
1	D	300[A]	ARG	3.7
1	D	410	ASP	3.6
1	D	218	LYS	3.5
1	D	243	TYR	3.5
1	A	214	ASP	3.5
1	A	216	GLU	3.4
1	D	358	GLU	3.3
1	A	215	THR	3.3
1	B	217	MET	3.2
1	C	262	THR	3.1
1	D	435	GLY	3.0
1	C	220	TYR	2.9
1	C	479	PHE	2.9
1	D	219	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	410	ASP	2.8
1	D	214	ASP	2.8
1	C	473	ALA	2.8
1	D	481	LYS	2.8
1	B	413	ARG	2.8
1	B	320	GLN	2.8
1	D	259	LEU	2.7
1	C	409	LYS	2.7
1	C	480	LYS	2.7
1	D	471	TYR	2.7
1	C	472	TYR	2.6
1	D	427	LEU	2.6
1	B	219	TYR	2.5
1	B	410	ASP	2.5
1	C	468	ILE	2.5
1	D	216	GLU	2.4
1	D	270	CYS	2.4
1	A	134	LYS	2.4
1	C	281	LEU	2.3
1	D	411	GLY	2.3
1	C	463	ASP	2.3
1	C	355	HIS	2.3
1	C	215	THR	2.3
1	D	254	PHE	2.3
1	C	475	GLN	2.3
1	C	471	TYR	2.3
1	D	230	PHE	2.2
1	C	316	GLN	2.2
1	B	252	THR	2.2
1	C	259	LEU	2.2
1	D	135	VAL	2.2
1	D	172	GLN	2.2
1	C	219	TYR	2.2
1	B	314	LEU	2.2
1	B	248	LEU	2.1
1	D	436	GLY	2.1
1	C	319	TYR	2.1
1	C	405	LEU	2.1
1	C	410	ASP	2.1
1	C	160	GLU	2.1
1	B	316	GLN	2.0
1	D	437	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	217	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	B	321[A]	16/17	0.81	0.17	82,86,90,95	13
1	PTR	B	321[B]	16/17	0.81	0.17	70,82,89,95	13
1	PTR	D	321[A]	16/17	0.84	0.15	67,81,87,89	13
1	PTR	D	321[B]	16/17	0.84	0.15	63,72,87,89	13
1	PTR	C	321[A]	16/17	0.87	0.13	60,73,77,80	13
1	PTR	C	321[B]	16/17	0.87	0.13	64,68,74,80	13
1	PTR	A	321[A]	16/17	0.87	0.14	52,70,73,77	13
1	PTR	A	321[B]	16/17	0.87	0.14	61,68,71,77	13

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	505	5/5	0.71	0.15	96,103,112,114	0
4	SO4	C	503	5/5	0.71	0.15	93,108,113,122	0
4	SO4	B	503	5/5	0.77	0.14	95,96,116,117	0
2	PG4	C	501	13/13	0.84	0.12	67,76,79,80	0
3	4H5	C	502	19/19	0.89	0.15	68,79,100,126	0
3	4H5	A	502	19/19	0.89	0.17	58,64,75,124	0
3	4H5	D	501	19/19	0.90	0.17	76,93,101,169	0
3	4H5	B	502	19/19	0.92	0.11	52,60,78,140	0
2	PG4	B	501	13/13	0.92	0.10	37,46,50,52	0

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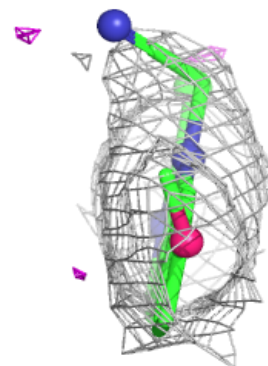
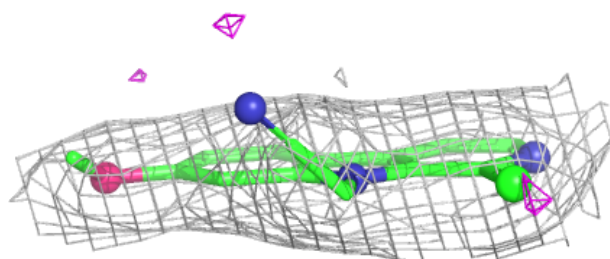
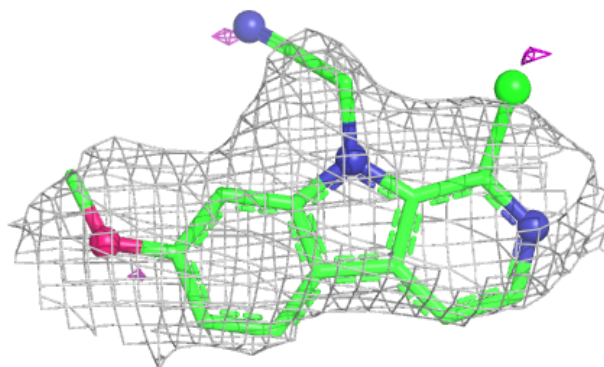
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PG4	A	501	13/13	0.93	0.10	38,42,46,48	0
4	SO4	B	504	5/5	0.93	0.08	75,82,89,90	0

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.

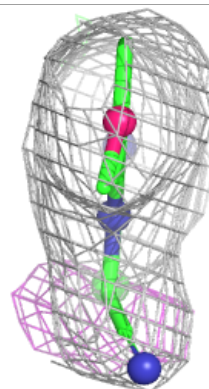
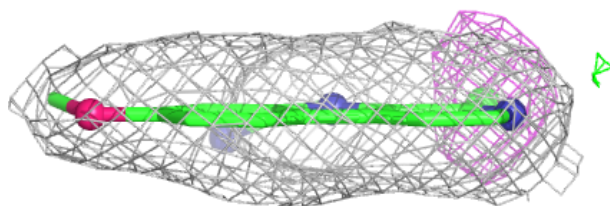
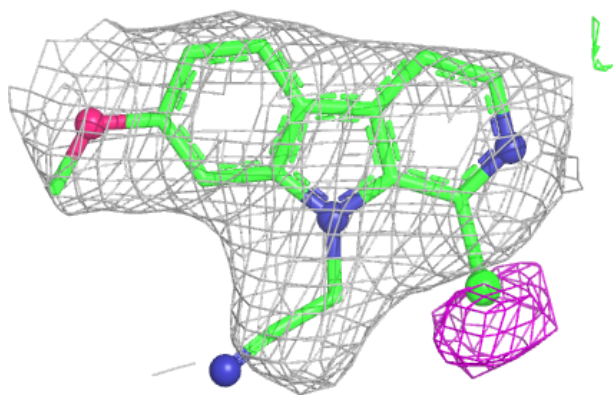
Electron density around 4H5 C 502:

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

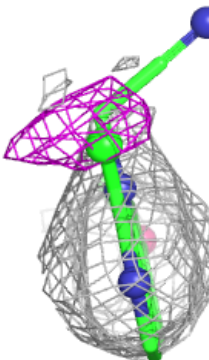
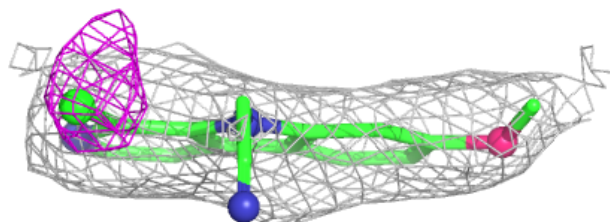
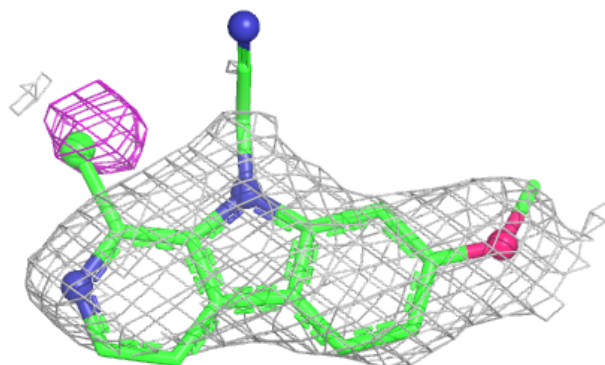


Electron density around 4H5 A 502:

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

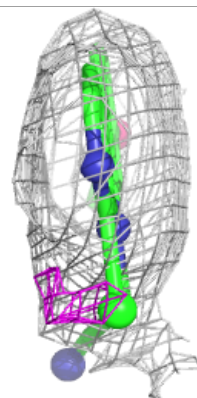
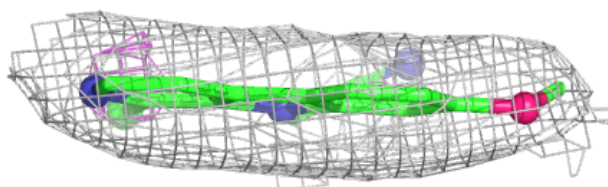
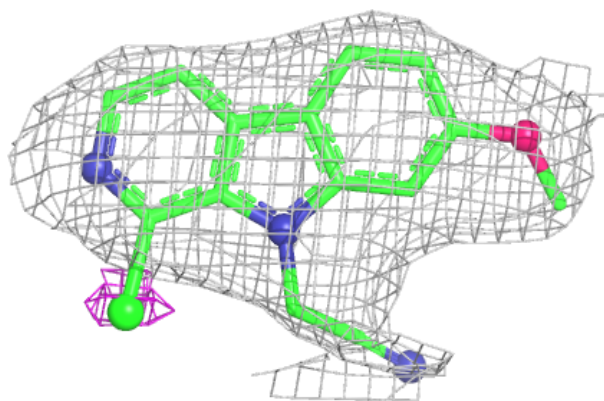
**Electron density around 4H5 D 501:**

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



Electron density around 4H5 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.