



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 12:19 pm BST

PDB ID : 4DAJ  
Title : Structure of the M3 Muscarinic Acetylcholine Receptor  
Authors : Kruse, A.C.; Hu, J.; Pan, A.C.; Arlow, D.H.; Rosenbaum, D.M.; Rosemond, E.; Green, H.F.; Liu, T.; Chae, P.S.; Dror, R.O.; Shaw, D.E.; Weis, W.I.; Wess, J.; Kobilka, B.  
Deposited on : 2012-01-12  
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

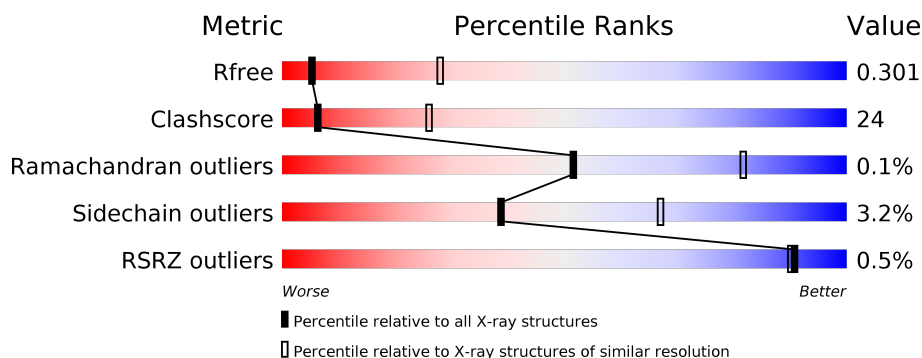
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	479	
1	B	479	
1	C	479	
1	D	479	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OHK	D	2000	-	-	X	-
3	PO4	A	2003	-	-	X	-
3	PO4	C	2001	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13589 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 Muscarinic acetylcholine receptor M3, Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3405	2223	566	596	20			
1	B	430	Total	C	N	O	S	0	0	0
			3330	2181	542	587	20			
1	C	430	Total	C	N	O	S	0	0	0
			3314	2164	545	585	20			
1	D	432	Total	C	N	O	S	0	0	0
			3386	2215	562	589	20			

There are 36 discrepancies between the modelled and reference sequences:

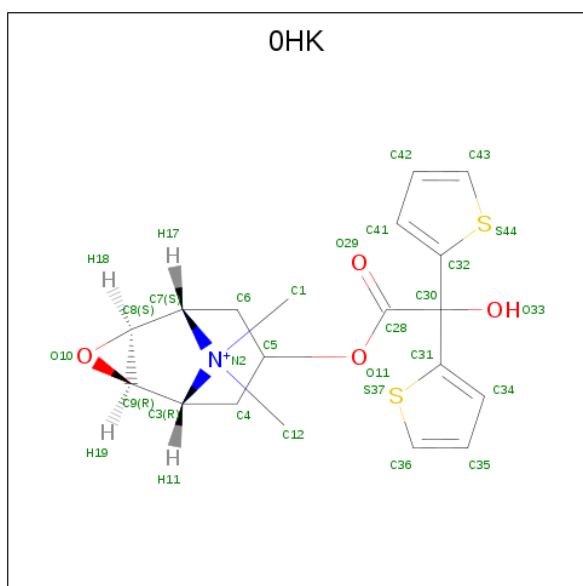
Chain	Residue	Modelled	Actual	Comment	Reference
A	56	GLY	-	EXPRESSION TAG	UNP P08483
A	1054	THR	CYS	ENGINEERED MUTATION	UNP P00720
A	1097	ALA	CYS	ENGINEERED MUTATION	UNP P00720
A	590	HIS	-	EXPRESSION TAG	UNP P08483
A	591	HIS	-	EXPRESSION TAG	UNP P08483
A	592	HIS	-	EXPRESSION TAG	UNP P08483
A	593	HIS	-	EXPRESSION TAG	UNP P08483
A	594	HIS	-	EXPRESSION TAG	UNP P08483
A	595	HIS	-	EXPRESSION TAG	UNP P08483
B	56	GLY	-	EXPRESSION TAG	UNP P08483
B	1054	THR	CYS	ENGINEERED MUTATION	UNP P00720
B	1097	ALA	CYS	ENGINEERED MUTATION	UNP P00720
B	590	HIS	-	EXPRESSION TAG	UNP P08483
B	591	HIS	-	EXPRESSION TAG	UNP P08483
B	592	HIS	-	EXPRESSION TAG	UNP P08483
B	593	HIS	-	EXPRESSION TAG	UNP P08483
B	594	HIS	-	EXPRESSION TAG	UNP P08483
B	595	HIS	-	EXPRESSION TAG	UNP P08483
C	56	GLY	-	EXPRESSION TAG	UNP P08483
C	1054	THR	CYS	ENGINEERED MUTATION	UNP P00720
C	1097	ALA	CYS	ENGINEERED MUTATION	UNP P00720

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Chain	Residue	Modelled	Actual	Comment	Reference
C	590	HIS	-	EXPRESSION TAG	UNP P08483
C	591	HIS	-	EXPRESSION TAG	UNP P08483
C	592	HIS	-	EXPRESSION TAG	UNP P08483
C	593	HIS	-	EXPRESSION TAG	UNP P08483
C	594	HIS	-	EXPRESSION TAG	UNP P08483
C	595	HIS	-	EXPRESSION TAG	UNP P08483
D	56	GLY	-	EXPRESSION TAG	UNP P08483
D	1054	THR	CYS	ENGINEERED MUTATION	UNP P00720
D	1097	ALA	CYS	ENGINEERED MUTATION	UNP P00720
D	590	HIS	-	EXPRESSION TAG	UNP P08483
D	591	HIS	-	EXPRESSION TAG	UNP P08483
D	592	HIS	-	EXPRESSION TAG	UNP P08483
D	593	HIS	-	EXPRESSION TAG	UNP P08483
D	594	HIS	-	EXPRESSION TAG	UNP P08483
D	595	HIS	-	EXPRESSION TAG	UNP P08483

- Molecule 2 is (1R,2R,4S,5S,7S)-7-{[hydroxy(dithiophen-2-yl)acetyl]oxy}-9,9-dimethyl-3-oxa-9-azoniatricyclo[3.3.1.0 2,4 ]nonane (three-letter code: 0HK) (formula: C<sub>19</sub>H<sub>22</sub>NO<sub>4</sub>S<sub>2</sub>).



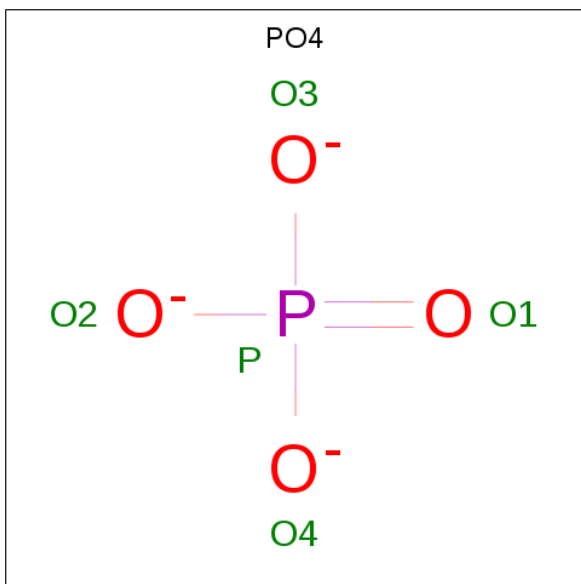
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	19	1	4	2		
2	B	1	Total	C	N	O	S	0	0
			26	19	1	4	2		
2	C	1	Total	C	N	O	S	0	0
			26	19	1	4	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			26	19	1	4	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

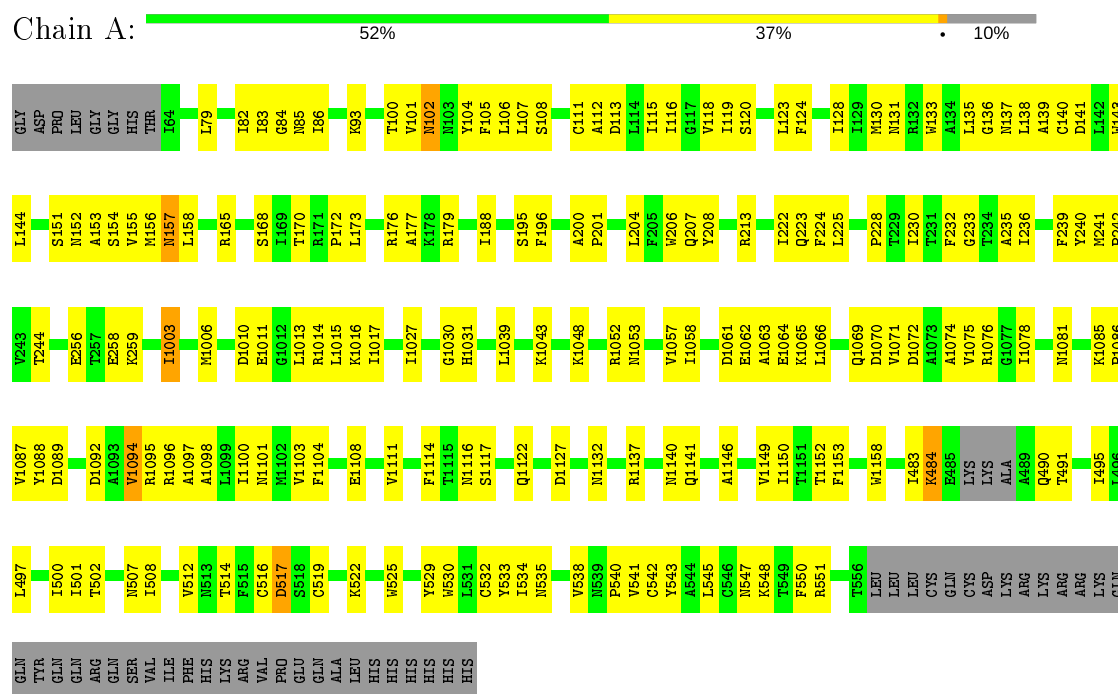


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

### 3 Residue-property plots

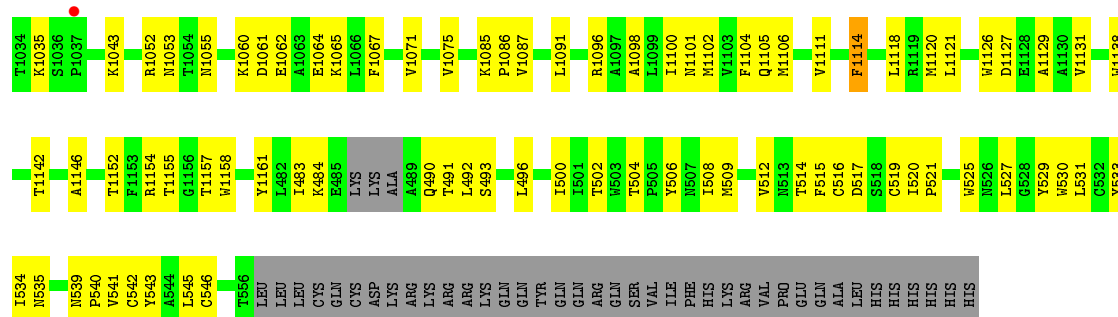
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Muscarinic acetylcholine receptor M3, Lysozyme

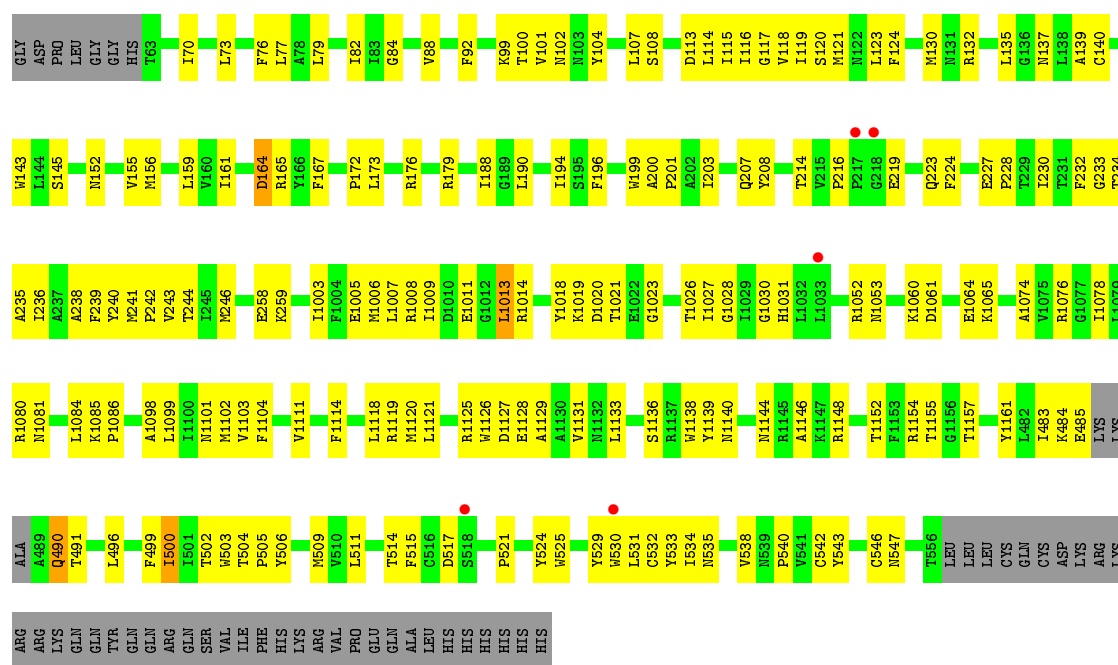


- Molecule 1: Muscarinic acetylcholine receptor M3, Lysozyme

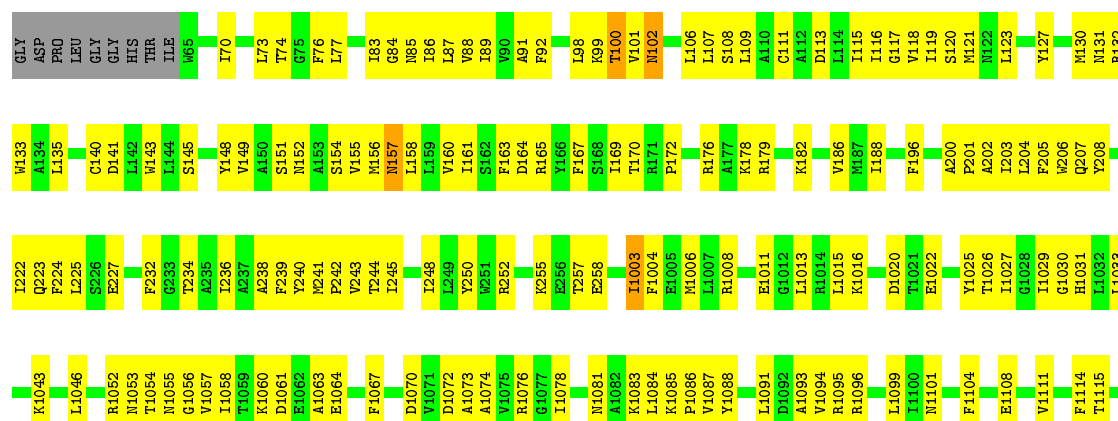




- Molecule 1: Muscarinic acetylcholine receptor M3, Lysozyme



- Molecule 1: Muscarinic acetylcholine receptor M3, Lysozyme





L1118		L1118
M1132		M1132
N1144		N1144
K1147		K1147
R1148		R1148
V1149		V1149
I1150		I1150
T1151		T1151
T1152		T1152
F1153		F1153
W1158		W1158
Y1161		Y1161
L482		L482
I483		I483
K484		K484
E485		E485
LYS		LYS
LYS		LYS
A488		A488
A489		A489
Q490		Q490
T491		T491
L492		L492
S493		S493
A494		A494
I495		I495
L496		L496
L497		L497
A498		A498
F499		F499
I500		I500
I501		I501
T502		T502
W503		W503
T504		T504
P505		P505
Y506		Y506
W507		W507
I508		I508
W509		W509
W510		W510
L511		L511
D517		D517
S518		S518
G519		G519
I520		I520
P521		P521
K522		K522
T523		T523
L527		L527
G528		G528
Y529		Y529
W530		W530

L531		L531
C532		C532
Y533		Y533
I534		I534
W535		W535
W538		W538
W539		W539
P540		P540
Y543		Y543
W547		W547
K548		K548
T549		T549
P550		P550
R551		R551
P554		P554
L559		L559
CYS		CYS
GLN		GLN
CYS		CYS
ASP		ASP
LYS		LYS
ARG		ARG
LYS		LYS
ARG		ARG
ARG		ARG
LYS		LYS
GLN		GLN
TYR		TYR
GLN		GLN
GLN		GLN
GLN		GLN
ARG		ARG
GLN		GLN
SER		SER
VAL		VAL
ILE		ILE
PHE		PHE
HIS		HIS
LYS		LYS
ARG		ARG
VAL		VAL
PRO		PRO
GLU		GLU
GLN		GLN
ALA		ALA
LEU		LEU
HIS		HIS
HIS		HIS
HIS		HIS
HIS		HIS
HIS		HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.77Å 61.31Å 176.91Å 85.87° 89.90° 84.90°	Depositor
Resolution (Å)	39.90 – 3.40 39.90 – 3.40	Depositor EDS
% Data completeness (in resolution range)	82.9 (39.90-3.40) 82.9 (39.90-3.40)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.251 , 0.303 0.242 , 0.301	Depositor DCC
$R_{free}$ test set	1277 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	13589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 0HK, PO4

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	0.30	0/3482	0.48	0/4738
1	B	0.29	0/3407	0.49	1/4655 (0.0%)
1	C	0.27	0/3391	0.45	0/4639
1	D	0.30	0/3465	0.50	1/4726 (0.0%)
All	All	0.29	0/13745	0.48	2/18758 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	CYS	CB-CA-C	6.17	122.73	110.40
1	D	519	CYS	CA-CB-SG	-6.07	103.07	114.00

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	3405	0	3451	159	0
1	B	3330	0	3304	153	0
1	C	3314	0	3243	152	0
1	D	3386	0	3391	195	0
2	A	26	0	22	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	22	7	0
2	C	26	0	22	7	0
2	D	26	0	22	11	0
3	A	20	0	0	2	0
3	B	5	0	0	0	0
3	C	10	0	0	3	0
3	D	15	0	0	0	0
All	All	13589	0	13477	655	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 24.

The worst 5 of 655 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:D:108:SER:HB2	1:D:188:ILE:HD13	1.36	1.08
1:D:484:LYS:H	1:D:484:LYS:HD3	1.24	0.98
1:D:120:SER:HA	1:D:143:TRP:HE1	1.27	0.96
1:C:152:ASN:HB2	2:C:2000:0HK:H6	1.50	0.94
2:D:2000:0HK:H20	2:D:2000:0HK:O10	1.70	0.91

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	425/479 (89%)	391 (92%)	33 (8%)	1 (0%)	47	78
1	B	426/479 (89%)	396 (93%)	30 (7%)	0	100	100
1	C	426/479 (89%)	389 (91%)	37 (9%)	0	100	100
1	D	428/479 (89%)	392 (92%)	36 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1705/1916 (89%)	1568 (92%)	136 (8%)	1 (0%)	51 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1094	VAL

### 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	360/416 (86%)	347 (96%)	13 (4%)	35 63
1	B	343/416 (82%)	334 (97%)	9 (3%)	46 72
1	C	336/416 (81%)	329 (98%)	7 (2%)	53 76
1	D	351/416 (84%)	336 (96%)	15 (4%)	29 59
All	All	1390/1664 (84%)	1346 (97%)	44 (3%)	39 67

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	517	ASP
1	C	1140	ASN
1	D	517	ASP
1	B	519	CYS
1	C	164	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	513	ASN
1	C	102	ASN
1	D	490	GLN
1	B	526	ASN

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Mol	Chain	Res	Type
1	B	535	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

14 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	$\# Z  > 2$
2	0HK	A	2000	-	28,30,30	1.81	8 (28%)	38,48,48	4.68	19 (50%)
3	PO4	A	2001	-	4,4,4	0.93	0	6,6,6	0.43	0
3	PO4	D	2003	-	4,4,4	0.88	0	6,6,6	0.46	0
3	PO4	A	2004	-	4,4,4	0.88	0	6,6,6	0.46	0
3	PO4	A	2003	-	4,4,4	0.91	0	6,6,6	0.45	0
2	0HK	B	2000	-	28,30,30	1.79	9 (32%)	38,48,48	4.85	20 (52%)
3	PO4	B	2001	-	4,4,4	0.94	0	6,6,6	0.47	0
3	PO4	D	2001	-	4,4,4	0.87	0	6,6,6	0.45	0
2	0HK	D	2000	-	28,30,30	1.75	7 (25%)	38,48,48	4.94	18 (47%)
3	PO4	C	2002	-	4,4,4	0.88	0	6,6,6	0.40	0
3	PO4	A	2002	-	4,4,4	0.94	0	6,6,6	0.42	0
3	PO4	D	2002	-	4,4,4	0.91	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	C	2001	-	4,4,4	1.01	0	6,6,6	0.27	0
2	0HK	C	2000	-	28,30,30	1.79	9 (32%)	38,48,48	5.02	20 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0HK	B	2000	-	-	2/10/55/55	0/6/5/5
2	0HK	A	2000	-	-	0/10/55/55	0/6/5/5
2	0HK	D	2000	-	-	2/10/55/55	0/6/5/5
2	0HK	C	2000	-	-	2/10/55/55	0/6/5/5

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	0HK	C1-N2	-4.43	1.42	1.51
2	D	2000	0HK	C1-N2	-4.06	1.43	1.51
2	A	2000	0HK	O11-C28	3.93	1.41	1.34
2	D	2000	0HK	O11-C28	3.72	1.41	1.34
2	B	2000	0HK	O11-C28	3.67	1.41	1.34

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	0HK	C35-C36-S37	-15.02	100.78	112.98
2	D	2000	0HK	C42-C43-S44	-14.87	100.91	112.98
2	C	2000	0HK	C42-C43-S44	-14.52	101.19	112.98
2	C	2000	0HK	C35-C36-S37	-14.05	101.57	112.98
2	A	2000	0HK	C42-C43-S44	-14.00	101.61	112.98

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2000	0HK	O29-C28-O11-C5
2	D	2000	0HK	O29-C28-O11-C5
2	B	2000	0HK	C30-C28-O11-C5
2	C	2000	0HK	O29-C28-O11-C5
2	D	2000	0HK	O29-C28-C30-C32

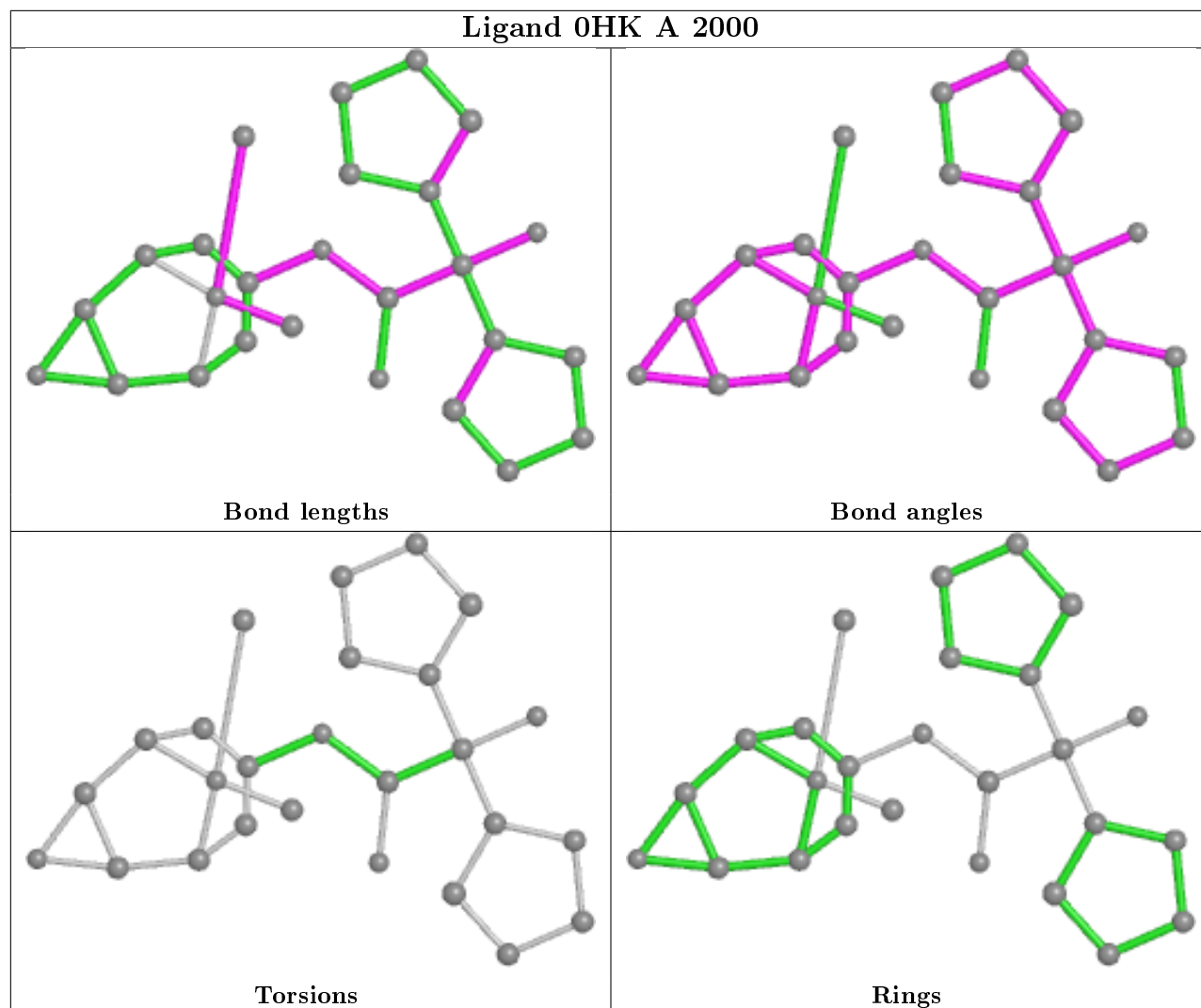
There are no ring outliers.

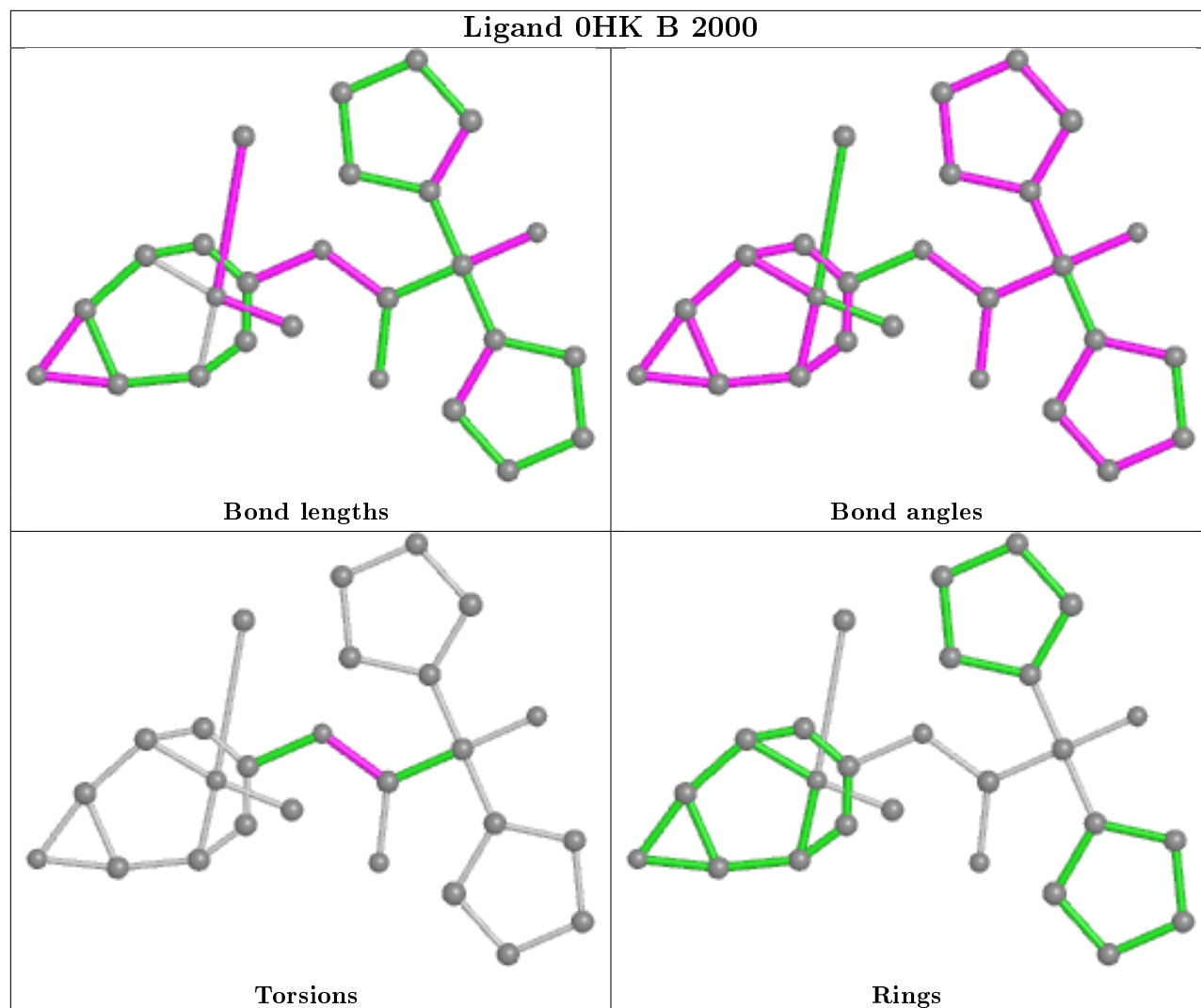
7 monomers are involved in 37 short contacts:

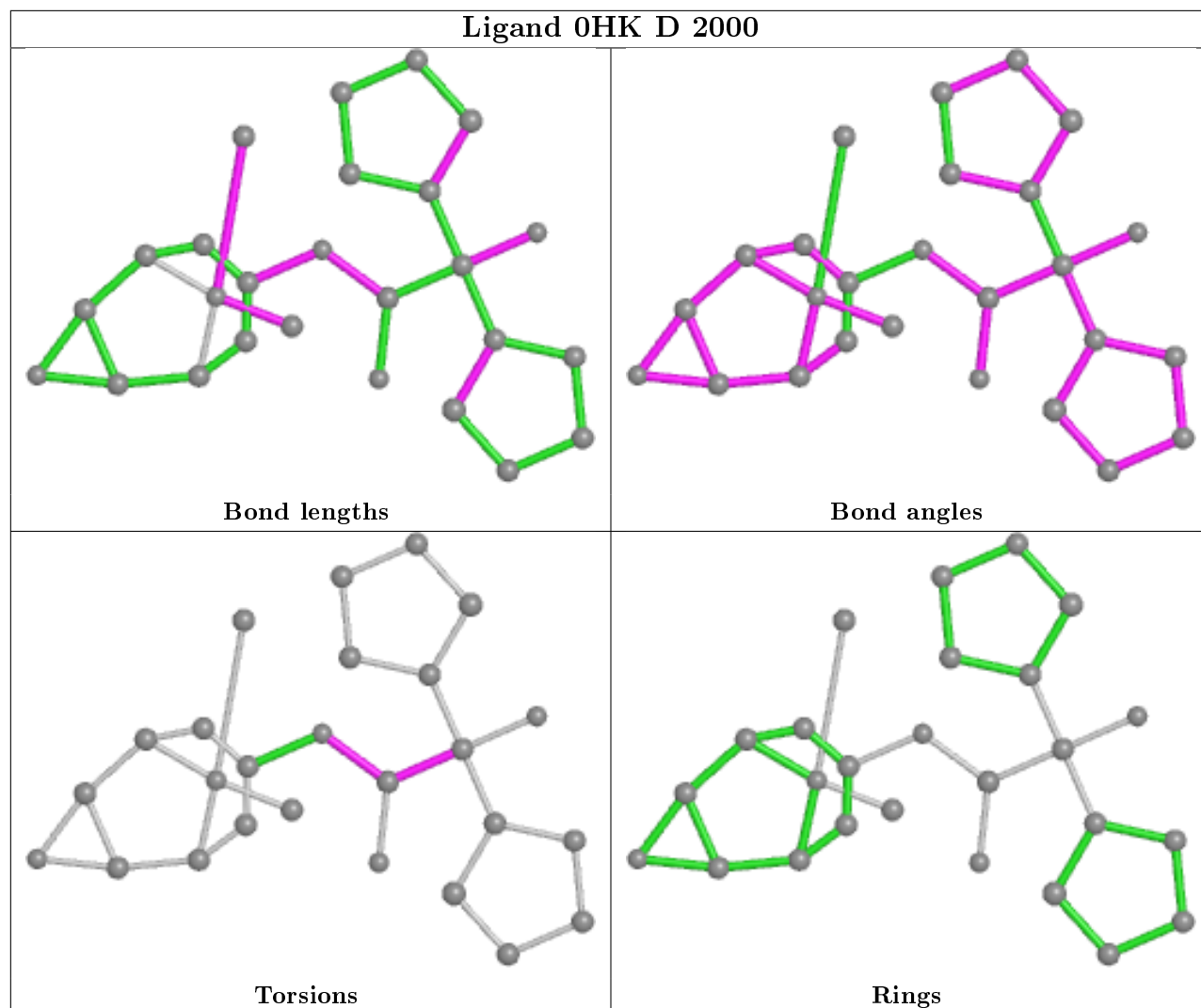
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	0HK	7	0
3	A	2003	PO4	2	0
2	B	2000	0HK	7	0
2	D	2000	0HK	11	0
3	C	2002	PO4	1	0
3	C	2001	PO4	2	0
2	C	2000	0HK	7	0

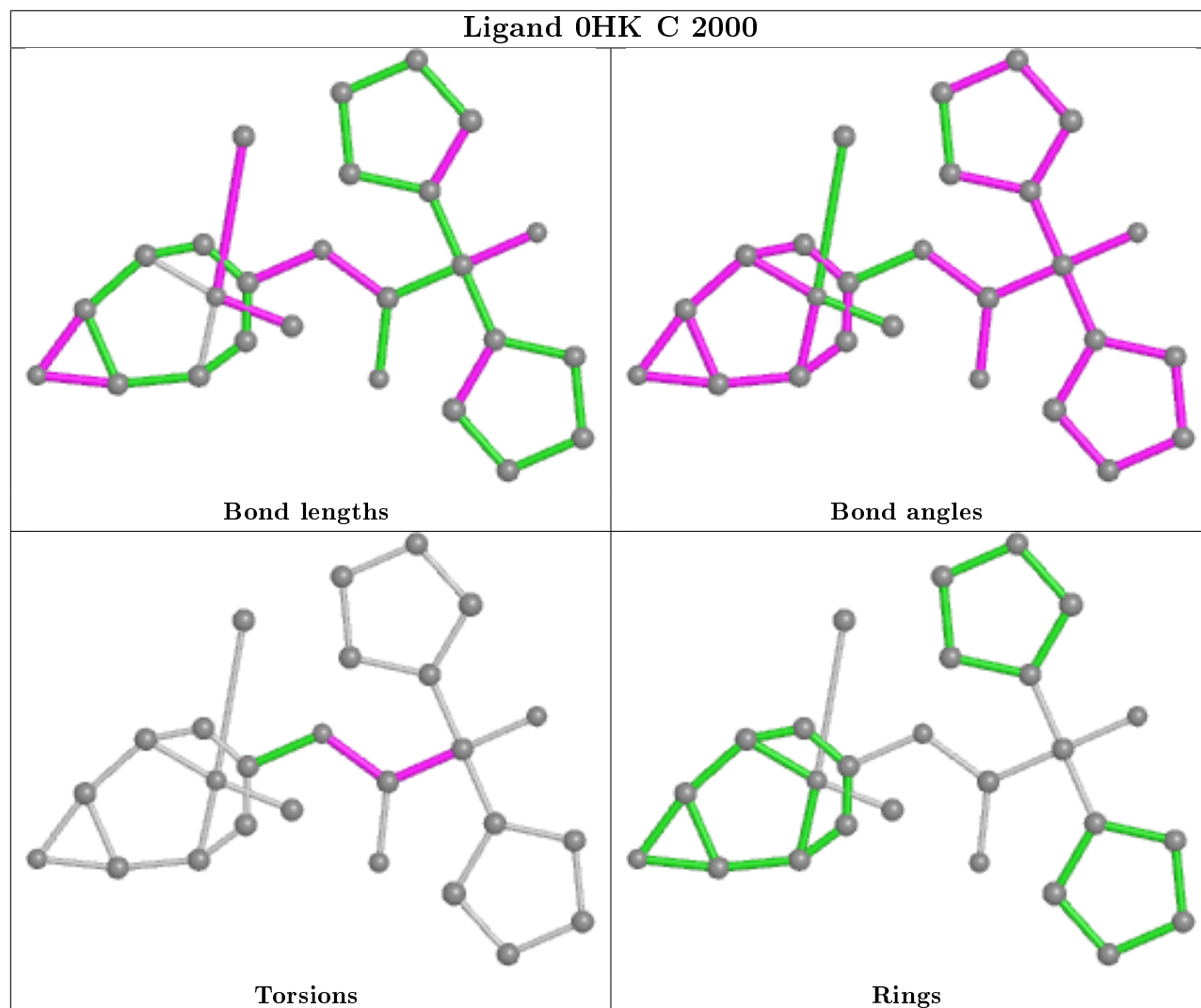
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	429/479 (89%)	-0.36	0 100 100	42, 71, 115, 153	0
1	B	430/479 (89%)	-0.30	3 (0%) 87 87	41, 92, 136, 172	0
1	C	430/479 (89%)	-0.23	5 (1%) 79 77	51, 103, 154, 183	0
1	D	432/479 (90%)	-0.36	0 100 100	40, 77, 124, 207	0
All	All	1721/1916 (89%)	-0.31	8 (0%) 91 90	40, 85, 136, 207	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1037	PRO	4.4
1	C	218	GLY	3.8
1	C	1033	LEU	3.4
1	C	530	TRP	2.9
1	C	518	SER	2.8

### 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](#)

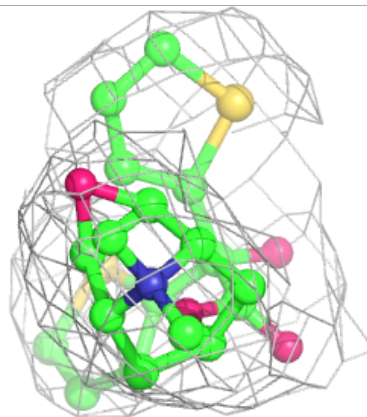
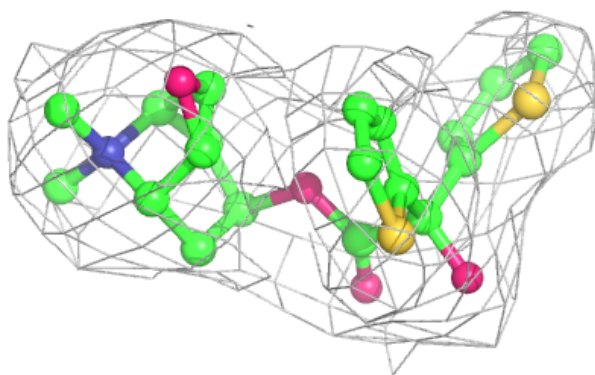
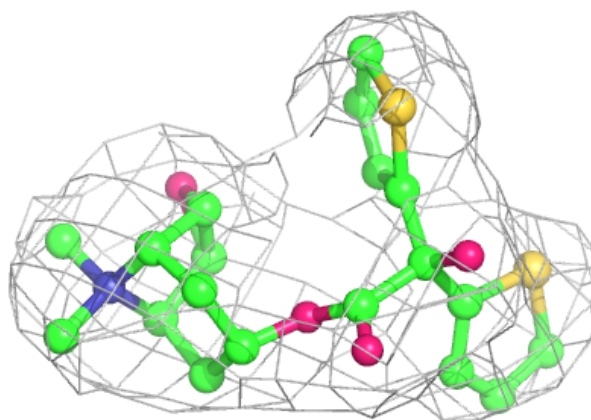
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	C	2002	5/5	0.81	0.17	121,127,142,152	0
3	PO4	A	2001	5/5	0.85	0.17	102,117,134,135	0
3	PO4	D	2002	5/5	0.91	0.12	113,113,122,133	0
3	PO4	D	2001	5/5	0.92	0.16	116,120,134,140	0
3	PO4	A	2003	5/5	0.93	0.19	111,114,136,138	0
3	PO4	B	2001	5/5	0.94	0.25	102,123,125,143	0
3	PO4	A	2002	5/5	0.95	0.17	87,88,94,107	0
3	PO4	D	2003	5/5	0.95	0.17	61,80,87,88	0
3	PO4	C	2001	5/5	0.95	0.18	94,95,117,118	0
3	PO4	A	2004	5/5	0.96	0.24	106,108,116,127	0
2	0HK	D	2000	26/26	0.97	0.20	62,73,80,85	0
2	0HK	B	2000	26/26	0.98	0.20	56,66,74,77	0
2	0HK	A	2000	26/26	0.98	0.20	54,58,64,72	0
2	0HK	C	2000	26/26	0.98	0.23	68,78,84,90	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.

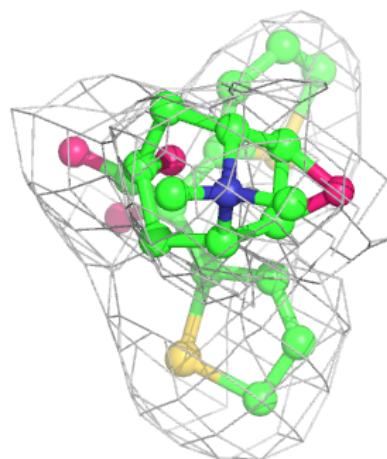
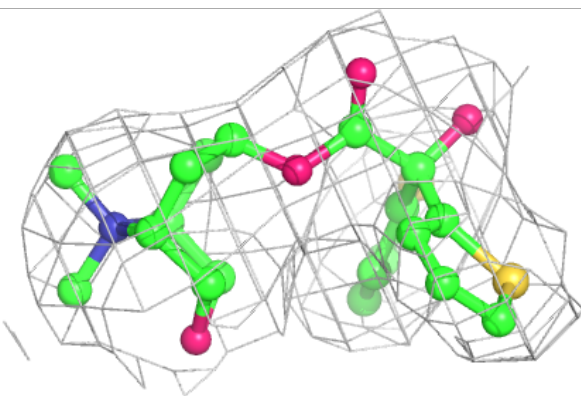
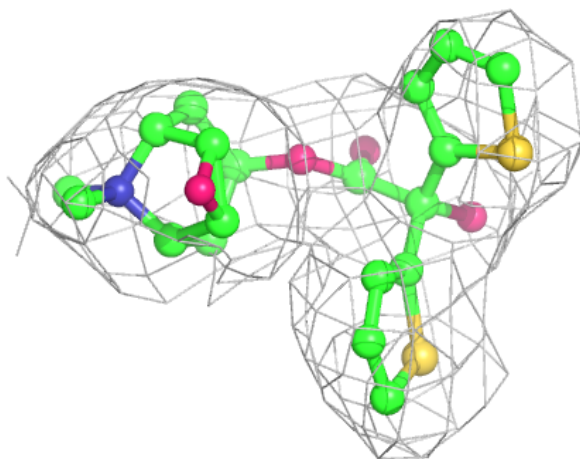
**Electron density around 0HK D 2000:**

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



**Electron density around 0HK B 2000:**

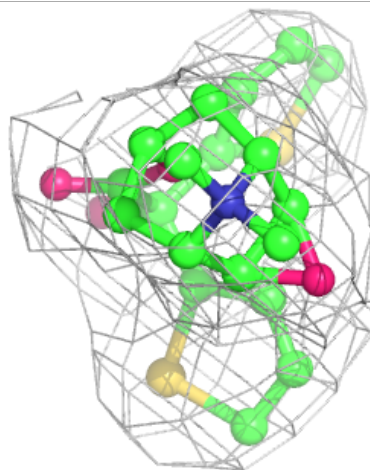
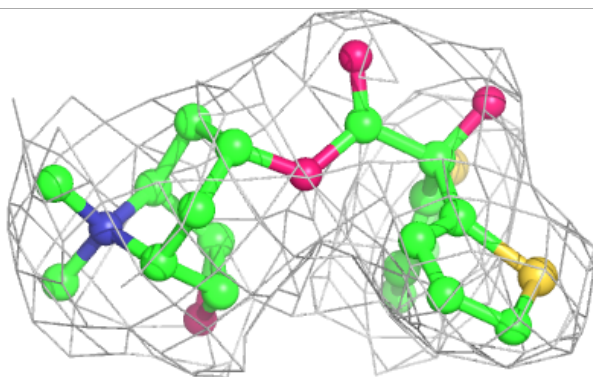
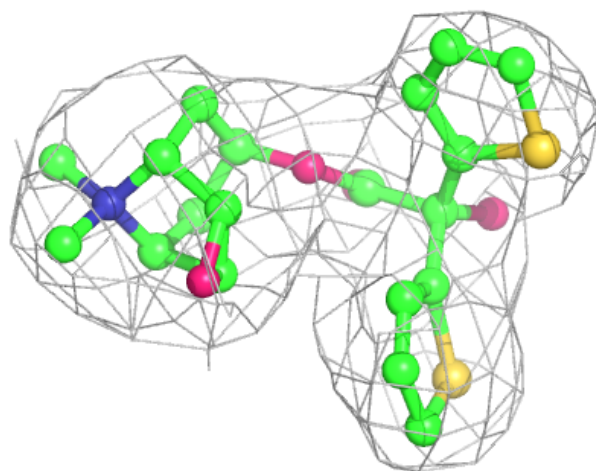
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





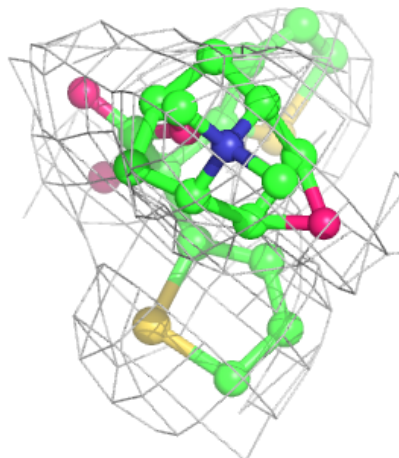
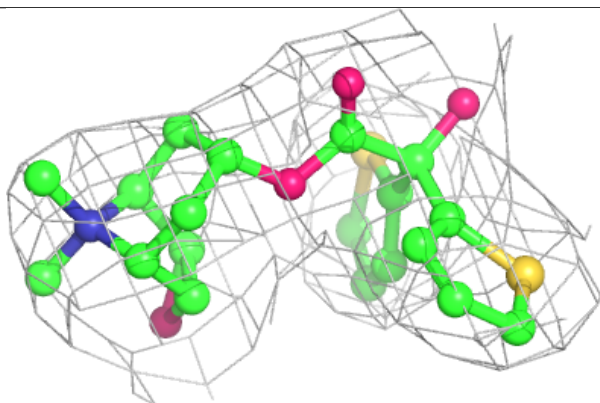
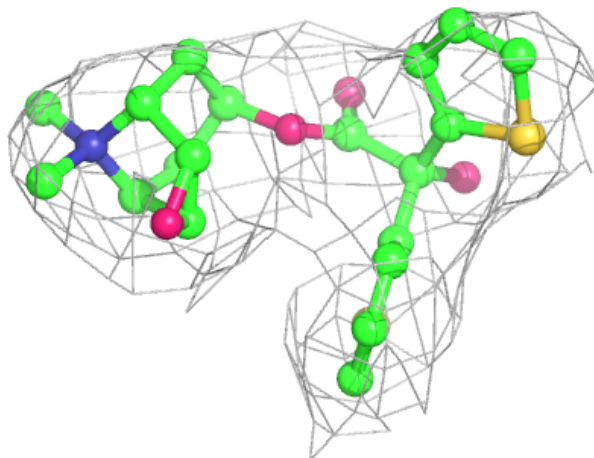
**Electron density around 0HK A 2000:**

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



**Electron density around 0HK C 2000:**

$2mF_o-DF_c$  (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.