



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:58 pm BST

PDB ID : 2BXB
Title : Human serum albumin complexed with oxyphenbutazone
Authors : Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Curry, S.
Deposited on : 2005-07-26
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

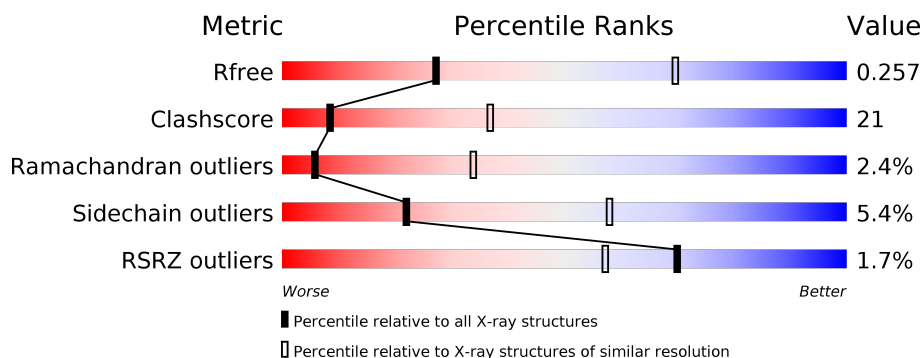
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>32%</div> <div>• •</div> </div> </div>
1	B	585	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>• •</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OPB	A	2001	X	-	-	-
2	OPB	B	2001	X	-	-	-

2 Entry composition [i](#)

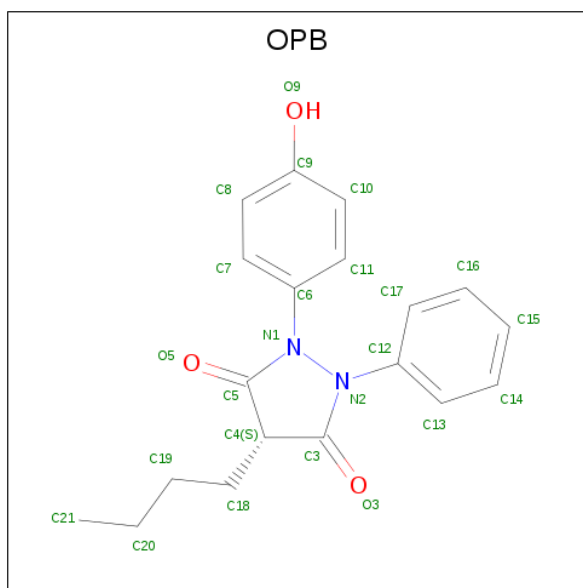
There are 2 unique types of molecules in this entry. The entry contains 8790 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4374	2754	732	847	41			
1	B	578	Total	C	N	O	S	0	0	0
			4368	2746	735	847	40			

- Molecule 2 is 4-BUTYL-1-(4-HYDROXYPHENYL)-2-PHENYLPYRAZOLIDINE-3,5-DIONE (three-letter code: OPB) (formula: $C_{19}H_{20}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	19	2	3		
2	B	1	Total	C	N	O	0	0
			24	19	2	3		

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 ($\text{RSRZ} > 2$). 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.

Chain A:

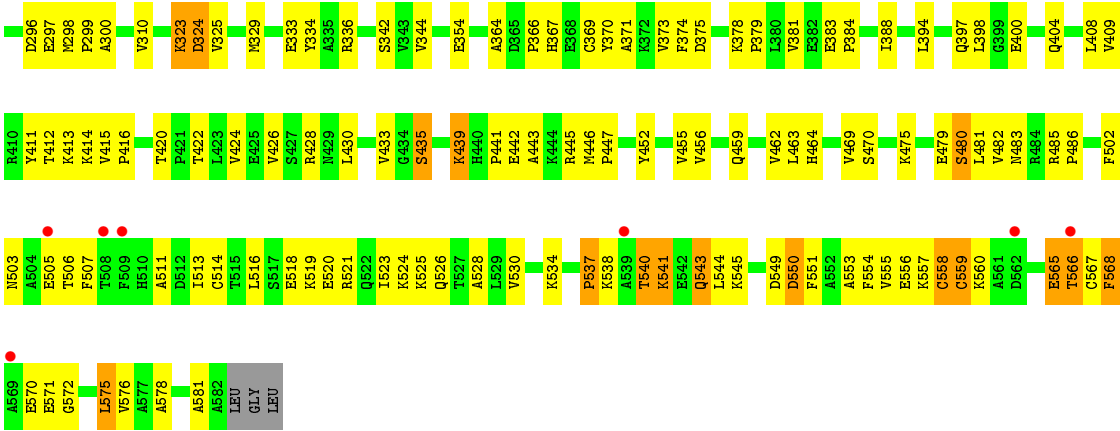
29% 64% 32%

Label	Value
V530	G434
P637	K436
K358	C437
A639	H440
T640	M446
K541	P447
E542	Y452
L544	V456
V547	Q459
F551	L460
F554	V462
V555	L463
C558	T467
D562	D471
E565	R472
T566	S480
C567	N483
F568	R494
A569	R485
E570	P486
E571	A492
G572	V493
L575	K500
V576	E501
A577	F502
A578	N503
A581	A504
A582	Y411
LEU	T506
GLY	F507
LEU	T508
	F509
	H510
	A511
	D512
	T515
	K519
	I523
	K524
	R525
	Q526
	T527
	A528
	E529
ASP	T236
ALA	D237
HIS	L238
LYS	T239
S5	K240
E56	E244
V7	C245
L14	E252
L22	R257
V23	L260
I25	I264
Q29	C265
Y30	Q268
L31	S272
C34	S273
P35	K274
F36	C279
E37	E280
D38	K281
H39	P282
L42	L283
V43	L284
V46	E285
F49	K286
C53	S287
E57	I290
S58	A291
A59	E294
E60	H295
N61	D296
K64	P299
S65	A300
L66	R306
L67	V310
H67	D314
T68	P315
L69	Y319
F70	K323
G71	D324
D72	V325
K73	W326
L74	R327
T79	A329
N87	K339
Q94	D340
R222	V342
F223	V343
P224	V344
	L345
	L349
	H367
	V370
	A371
	K372
	V373
	F374
	D375
	K378
	P379
	L380
	V381
	E382
	E383
	P384
	I388
	L394
	Q397
	L398
	G399
	E400
	O404
	H405
	L408
	V409
	R410
	Y411
	T412
	R413
	K414
	V415
	P416
	Q417
	T420
	P421
	V424
	E425
	V426
	S427
	R428
	H429
	L430
	V432

Chain B:

29% 59% 36%

ASP AHA HIS LYS SS R9 D13 L14 G15 E16 F19 K20 A21 L22 V23 L24 L25 A26 F27 A28 Q29 Y30 L31 Q32 Q33 C34 P35 F36 E37 D38 B39 V40 V41 L42 V43 V46 T47 E48 F49 A50 K51 T52 C53 Y54 A55 D56 E57 S58 A59 E60 R61 C62 H67 E70 C75 V77 A78 T79 L80 R81 E82 T83 Y84 G85 A88 R89 N90 E90 C101 F102 L103 Q104 H105 K106 P110 R114 P118 E119 V120 L139 C245 C246 E247 R257 L260 A261 L264 S272 K276 P282 L283 L284 E285 K286 S287 E288 C289 A291 C292 P293



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.16Å 55.50Å 120.51Å 81.33° 90.52° 65.38°	Depositor
Resolution (Å)	22.88 – 3.20 22.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (22.88-3.20) 97.9 (22.88-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.23Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.276 0.213 , 0.257	Depositor DCC
R_{free} test set	1005 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8790	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OPB

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	0.33	0/4461	0.60	2/6055 (0.0%)
1	B	0.32	0/4452	0.59	2/6035 (0.0%)
All	All	0.32	0/8913	0.59	4/12090 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	CYS	CA-CB-SG	10.66	133.18	114.00
1	B	514	CYS	CA-CB-SG	-9.17	97.49	114.00
1	A	558	CYS	CA-CB-SG	8.13	128.63	114.00
1	A	567	CYS	CA-CB-SG	-5.18	104.67	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	4374	0	4064	183	0
1	B	4368	0	4075	169	0
2	A	24	0	18	6	0
2	B	24	0	18	5	0
All	All	8790	0	8175	352	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 21.

The worst 5 of 352 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:A:554:PHE:HB2	1:A:575:LEU:HD22	1.45	0.99
1:B:257:ARG:NH1	1:B:287:SER:HB3	1.82	0.95
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.34	0.92
1:A:67:HIS:HB3	1:A:98:ARG:HH21	1.38	0.87
1:A:117:ARG:HH12	1:A:182:LEU:HB3	1.43	0.84

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	576/585 (98%)	504 (88%)	58 (10%)	14 (2%)	6	34
1	B	576/585 (98%)	495 (86%)	67 (12%)	14 (2%)	6	34
All	All	1152/1170 (98%)	999 (87%)	125 (11%)	28 (2%)	6	34

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	300	ALA
1	A	315	VAL
1	A	504	ALA
1	A	510	HIS

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	451/511 (88%)	428 (95%)	23 (5%)	24	60
1	B	450/511 (88%)	424 (94%)	26 (6%)	20	55
All	All	901/1022 (88%)	852 (95%)	49 (5%)	22	58

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	568	PHE
1	B	179	LEU
1	B	558	CYS
1	B	56	ASP
1	B	204	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	404	GLN
1	A	464	HIS
1	B	318	ASN
1	A	397	GLN
1	B	385	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	OPB	B	2001	-	24,26,26	1.95	8 (33%)	25,36,36	0.97	1 (4%)
2	OPB	A	2001	-	24,26,26	2.01	6 (25%)	25,36,36	0.99	2 (8%)

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	OPB	B	2001	-	1/1/5/5	2/12/32/32	0/3/3/3
2	OPB	A	2001	-	1/1/5/5	1/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	OPB	N1-N2	4.42	1.49	1.42
2	B	2001	OPB	N1-N2	3.79	1.48	1.42
2	B	2001	OPB	C7-C6	3.54	1.46	1.39
2	A	2001	OPB	C7-C8	3.47	1.45	1.38
2	A	2001	OPB	C11-C6	3.21	1.45	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	OPB	C11-C10-C9	2.25	122.35	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	OPB	C10-C11-C6	2.17	123.18	120.32
2	A	2001	OPB	C8-C7-C6	2.04	123.01	120.32

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2001	OPB	C4
2	A	2001	OPB	C4

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	OPB	C19-C18-C4-C5
2	B	2001	OPB	C18-C19-C20-C21
2	A	2001	OPB	C19-C18-C4-C3

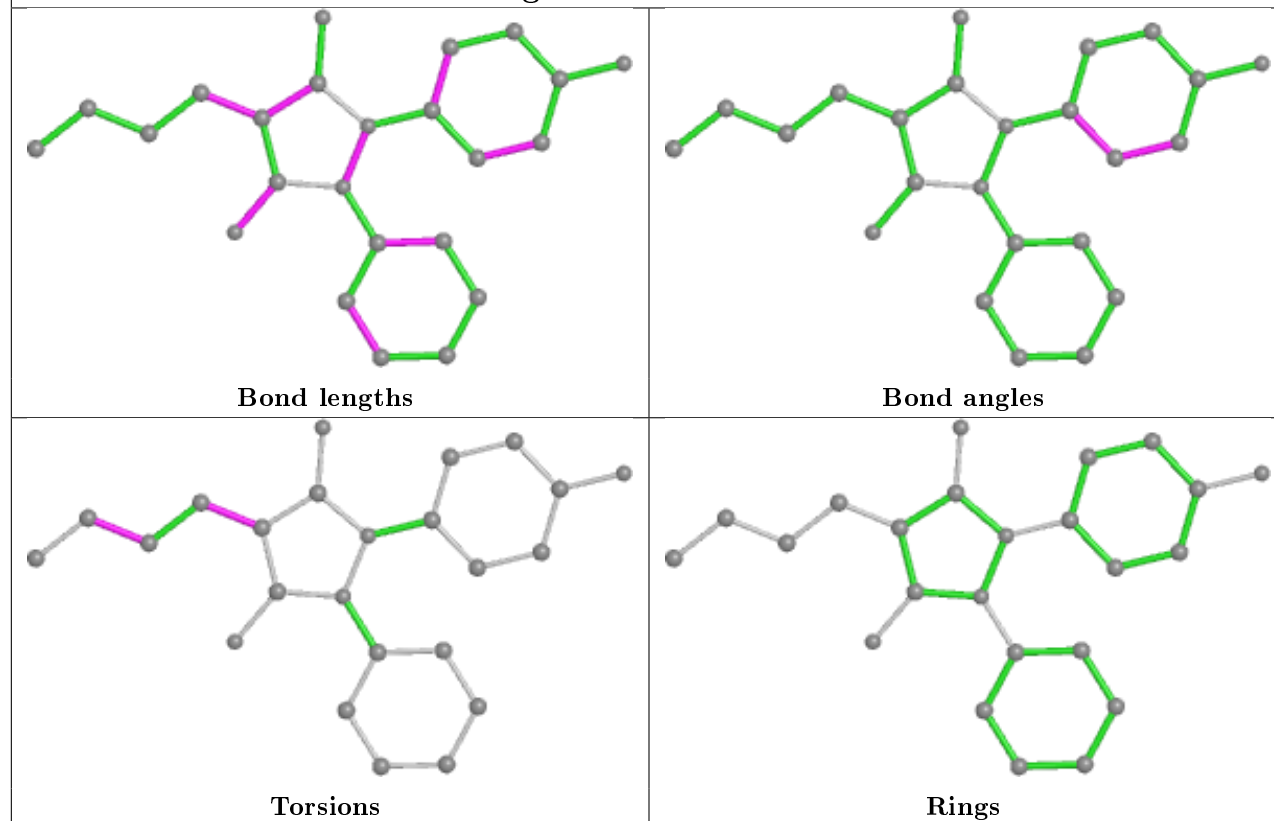
There are no ring outliers.

2 monomers are involved in 11 short contacts:

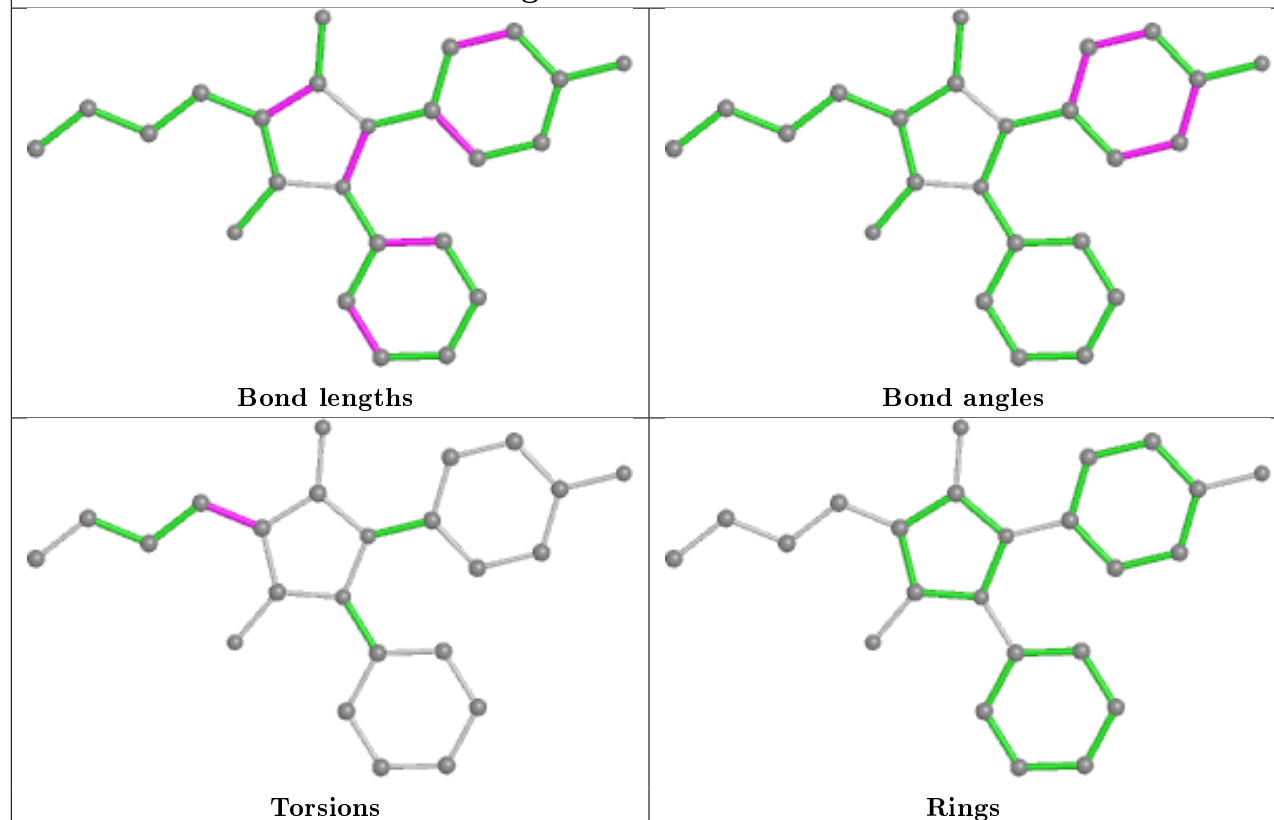
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	OPB	5	0
2	A	2001	OPB	6	0

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 OPB B 2001



Ligand OPB A 2001



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	578/585 (98%)	-0.41	9 (1%) 72 59	28, 65, 134, 150	0
1	B	578/585 (98%)	-0.36	11 (1%) 66 53	25, 67, 140, 153	0
All	All	1156/1170 (98%)	-0.38	20 (1%) 70 57	25, 66, 137, 153	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	562	ASP	4.8
1	B	508	THR	4.6
1	A	578	ALA	4.5
1	A	510	HIS	4.2
1	A	506	THR	4.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

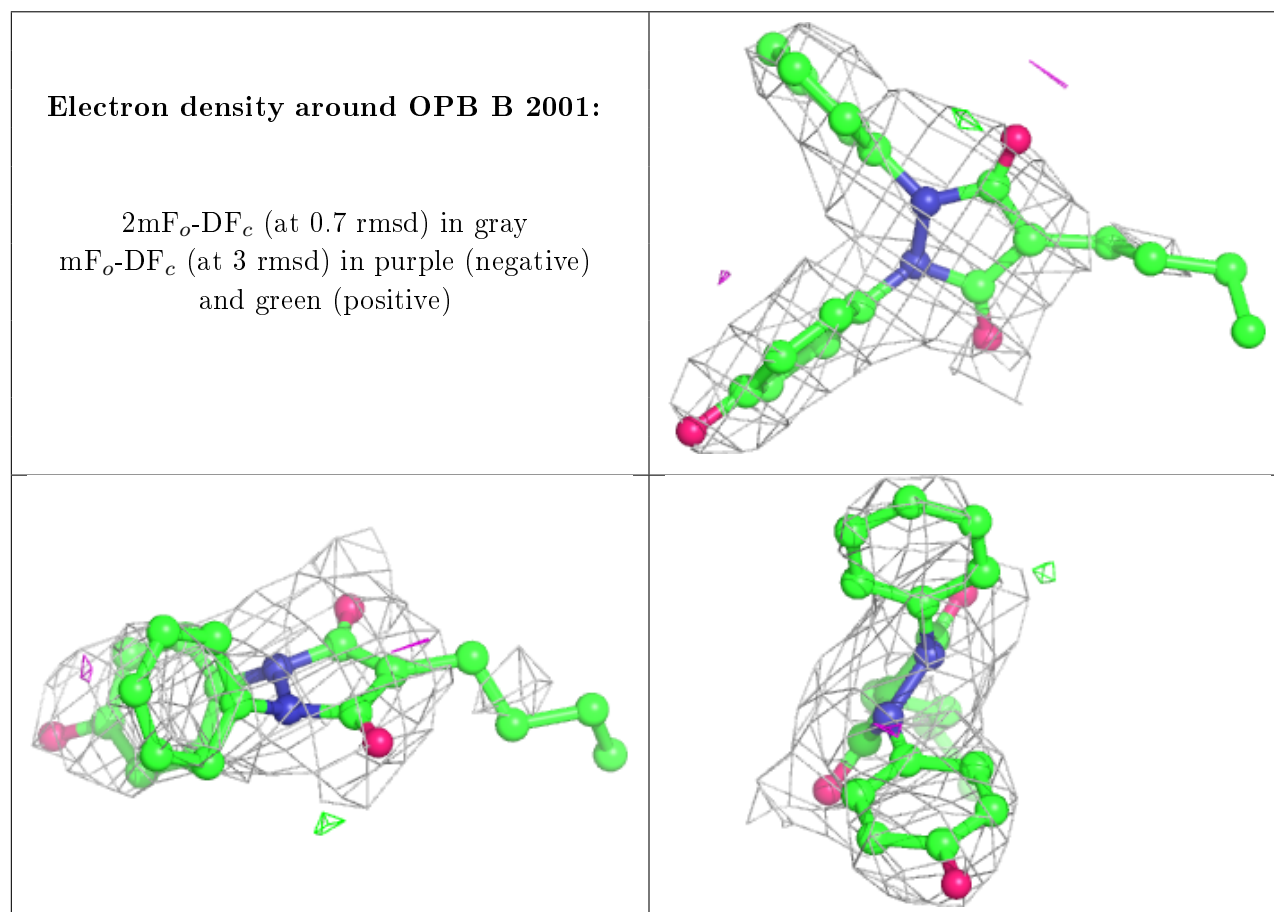
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

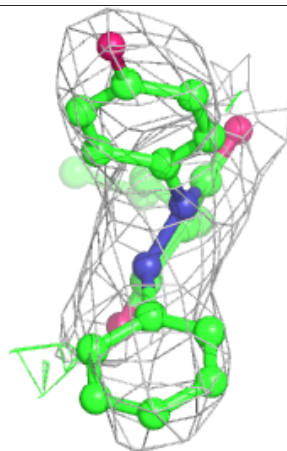
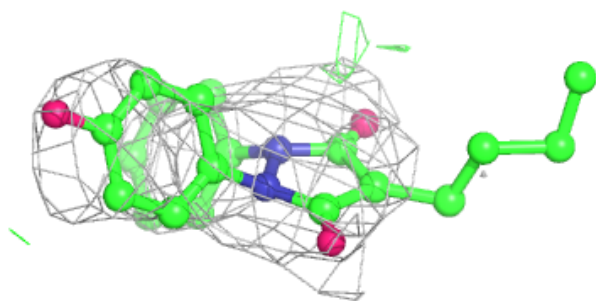
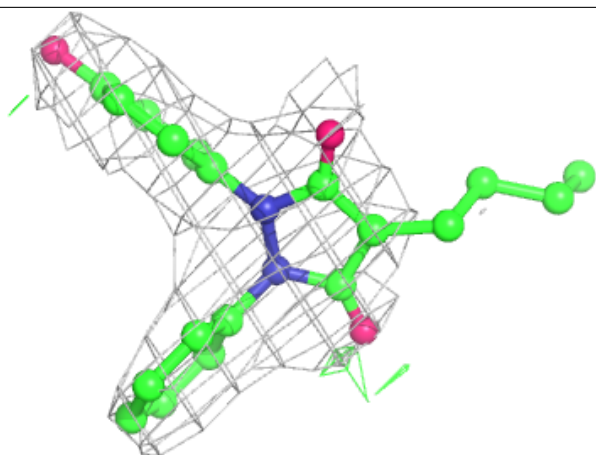
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OPB	B	2001	24/24	0.90	0.26	79,82,88,92	0
2	OPB	A	2001	24/24	0.92	0.25	73,77,83,86	0

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 OPB A 2001:

$2mF_o-DF_c$ (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.