

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 05:37 pm BST

PDB ID	:	2WF3
Title	:	Human BACE-1 in complex with 6-(ethylamino)-N-((1S,2R)-2-hydroxy-3-(((
		3-(methyloxy)phenyl)methyl)amino)-1-(phenylmethyl)propyl)-1-methyl-1, 3,
		4,5-tetrahydro- $2,1$ -benzothiazepine- 8 -carboxamide $2,2$ -dioxide
Authors	:	Charrier, N.; Clarke, B.; Demont, E.; Dingwall, C.; Dunsdon, R.; Hawkins,
		J.; Hubbard, J.; Hussain, I.; Maile, G.; Matico, R.; Mosley, J.; Naylor, A.;
		O'Brien, A.; Redshaw, S.; Rowland, P.; Soleil, V.; Smith, K.J.; Sweitzer, S.;
		Theobald, P.; Vesey, D.; Walter, D.S.; Wayne, G.
Deposited on	:	2009-04-02
Resolution	:	2.08 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 following versions of software and data (see references (1)) were used in the production of this report:

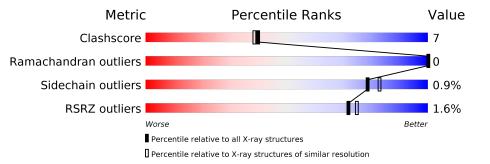
$\begin{array}{rcl} \mathrm{Mogul} &:& 1.8.5 \ (274361), \ \mathrm{CSD} \ \mathrm{as541be} \ (2020) \\ \mathrm{Xtriage} \ (\mathrm{Phenix}) &:& 1.13 \\ \mathrm{EDS} &:& 2.11 \\ \mathrm{buster-report} &:& 1.1.7 \ (2018) \\ \mathrm{Percentile} \ \mathrm{statistics} &:& 20191225.v01 \ (\mathrm{using} \ \mathrm{entries} \ \mathrm{in} \ \mathrm{the} \ \mathrm{PDB} \ \mathrm{archive} \ \mathrm{Decen} \\ \mathrm{Refmac} &:& 5.8.0158 \\ \mathrm{CCP4} &:& 7.0.044 \ (\mathrm{Gargrove}) \\ \mathrm{Ideal \ geometry} \ (\mathrm{proteins}) &:& \mathrm{Engh} \ \& \ \mathrm{Huber} \ (2001) \\ \mathrm{Ideal \ geometry} \ (\mathrm{DNA, RNA}) &:& \mathrm{Parkinson \ et \ al.} \ (1996) \\ \mathrm{Validation \ Pinoling} \ (wwPDB \ \mathrm{VP}) &:& 2.11 \end{array}$	ember 25th 2019):
Validation Pipeline (wwPDB-VP) : 2.11	

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 2.08 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 <=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				
			2%				
1	А	392	83%	12%	·		

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	\mathbf{Res}	Chirality	Geometry	Clashes	Electron density
3	GOL	А	2501	-	-	Х	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3345 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.

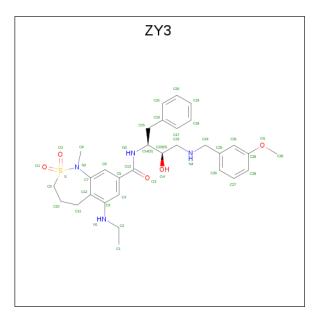
• Molecule 1 is a protein called BETA-SECRETASE 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	375	Total 2991	C 1912	N 498	O 567	S 14	0	7	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLN	ASN	engineered mutation	UNP P56817
A	172	GLN	ASN	engineered mutation	UNP P56817
A	223	GLN	ASN	engineered mutation	UNP P56817
А	354	GLN	ASN	engineered mutation	UNP P56817

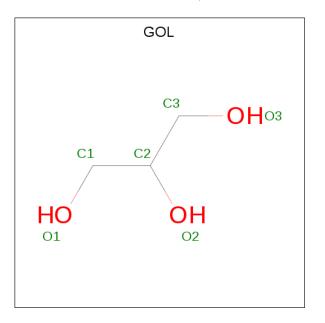
• Molecule 2 is N-{(1S,2R)-1-BENZYL-2-HYDROXY-3-[(3-METHOXYBENZYL)AMINO]P ROPYL}-6-(ETHYLAMINO)-1-METHYL-1,3,4,5-TETRAHYDRO-2,1-BENZOTHIAZEPI NE-8-CARBOXAMIDE 2,2-DIOXIDE (three-letter code: ZY3) (formula: C₃₁H₄₀N₄O₅S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
0	Λ	1	Total	С	Ν	Ο	S	0	0
	А	1	41	31	4	5	1	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

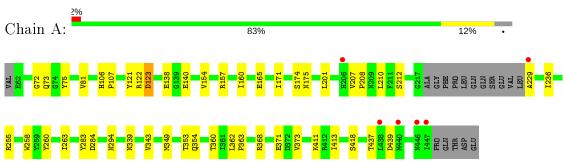
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	289	Total O 289 289	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: BETA-SECRETASE 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	48.45Å 76.87Å 104.48Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.90 - 2.08	Depositor
Resolution (A)	38.16 - 2.08	EDS
% Data completeness	99.3 (61.90-2.08)	Depositor
(in resolution range)	94.5(38.16-2.08)	EDS
R _{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.28 (at 2.08 \text{\AA})$	Xtriage
Refinement program	REFMAC 5	Depositor
D D.	0.164 , 0.217	Depositor
R, R_{free}	0.172 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	17.5	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 61.6	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	0.95	EDS
Total number of atoms	3345	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: GOL, ZY3 $\,$

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.90	0/3065	0.86	$4/4167 \ (0.1\%)$	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	157	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	А	157	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	А	210	LEU	CA-CB-CG	6.05	129.22	115.30
1	А	123	ASP	CB-CG-OD1	5.24	123.02	118.30

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	А	2991	0	2897	44	0
2	А	41	0	40	0	0
3	А	24	0	32	9	0
4	А	289	0	0	5	0
All	All	3345	0	2969	44	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 7.

All (44) close contacts within	the same	$\operatorname{asymmetric}$	unit ar	re listed	below,	sorted	by their	clash
magnitude.								

Atom 1	Atom 0	Interatomic	Clash
Atom-1	Atom-2	$distance (m \AA)$	overlap (Å)
1:A:72:GLY:H	3:A:2500:GOL:H2	1.21	1.00
1:A:353:THR:HG22	1:A:354:GLN:HG2	1.61	0.82
1:A:343:VAL:CG1	1:A:360[B]:THR:HG23	2.10	0.81
1:A:354:GLN:HE21	1:A:437:THR:HG23	1.47	0.79
1:A:343:VAL:HG13	1:A:360[B]:THR:CG2	2.15	0.76
1:A:72:GLY:N	3:A:2500:GOL:H2	1.98	0.76
1:A:343:VAL:HG13	1:A:360[B]:THR:HG23	1.69	0.73
1:A:343:VAL:CG1	1:A:360[B]:THR:CG2	2.67	0.72
1:A:354:GLN:O	1:A:437:THR:HG22	1.95	0.65
1:A:349:MET:HE1	4:A:2283:HOH:O	2.00	0.60
1:A:75:TYR:CE1	3:A:2500:GOL:H31	2.36	0.59
1:A:354:GLN:NE2	1:A:437:THR:HG23	2.17	0.58
1:A:263:ILE:HG13	1:A:349:MET:HE3	1.86	0.58
1:A:229:ALA:HB2	1:A:371:GLU:HG2	1.85	0.57
1:A:368:ARG:HH21	3:A:2501:GOL:H11	1.69	0.57
1:A:373[B]:VAL:HG23	4:A:2243:HOH:O	2.07	0.54
1:A:121:TYR:OH	4:A:2052:HOH:O	2.18	0.53
1:A:354:GLN:NE2	1:A:439:ASP:O	2.43	0.52
1:A:368:ARG:HH21	3:A:2501:GOL:C1	2.22	0.52
1:A:138:GLU:HG2	1:A:165:GLU:HB3	1.92	0.51
1:A:81[B]:VAL:HG11	1:A:160:ILE:HD13	1.92	0.51
1:A:154:VAL:HG21	1:A:201:LEU:CD1	2.42	0.49
1:A:343:VAL:HG11	1:A:360[B]:THR:CG2	2.43	0.48
1:A:368:ARG:NH2	3:A:2501:GOL:C1	2.77	0.48
1:A:263:ILE:HG21	1:A:349:MET:CE	2.43	0.48
1:A:362:LEU:HB3	1:A:363:PRO:HD2	1.96	0.48
1:A:263:ILE:HG21	1:A:349:MET:HE3	1.97	0.47
1:A:343:VAL:HG22	1:A:362:LEU:HD22	1.96	0.47
1:A:294:ASN:OD1	3:A:2501:GOL:H2	2.16	0.46
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.49	0.46
1:A:212[A]:SER:OG	1:A:236:ILE:HB	2.17	0.45
1:A:73:GLN:OE1	1:A:174:SER:HA	2.18	0.44
1:A:349:MET:CE	4:A:2283:HOH:O	2.61	0.44
1:A:368:ARG:NH2	3:A:2501:GOL:H12	2.33	0.43
1:A:339:ASN:ND2	4:A:2216:HOH:O	2.52	0.43
1:A:283:TYR:HA	1:A:284:ASP:HA	1.83	0.43
1:A:411:LYS:HB3	1:A:411:LYS:HE2	1.86	0.42
1:A:123:ASP:OD1	1:A:140:GLU:OE2	2.38	0.42

Continued on next page...



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:260:TYR:HB3	1:A:413[B]:ILE:HD11	2.02	0.42	
1:A:368:ARG:NH2	3:A:2501:GOL:H11	2.34	0.41	
1:A:207:VAL:HA	1:A:208:PRO:HD3	1.95	0.41	
1:A:171:ILE:HB	1:A:174:SER:HB3	2.02	0.41	
1:A:255:ARG:HD2	1:A:263:ILE:HD11	2.02	0.41	
1:A:174:SER:O	1:A:175:ASN:HB2	2.21	0.40	

Continued from previous page...

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	А	378/392~(96%)	367~(97%)	11 (3%)	0	100 100	

There are no Ramachandran outliers to report.

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	А	325/335~(97%)	322~(99%)	3~(1%)	78 83		

All (3) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	122	ARG
1	А	258	TRP
1	А	418	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	89	ASN
1	А	327	GLN
1	А	339	ASN
1	А	354	GLN
1	А	355	GLN
1	А	446	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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		
	туре				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	А	2502	-	5, 5, 5	0.41	0	5,5,5	0.69	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
	туре	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	GOL	А	2501	-	5, 5, 5	0.77	0	$5,\!5,\!5$	1.03	0
3	GOL	А	2500	-	5, 5, 5	0.21	0	$5,\!5,\!5$	1.02	0
3	GOL	А	2503	-	5, 5, 5	0.44	0	5, 5, 5	0.52	0
2	ZY3	А	2000	-	40,44,44	1.00	2(5%)	49,61,61	1.35	<u>6 (12%)</u>

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	GOL	А	2502	-	-	4/4/4/4	-
3	GOL	А	2501	-	-	4/4/4/4	-
3	GOL	А	2500	-	-	2/4/4/4	-
3	GOL	А	2503	-	-	4/4/4/4	-
2	ZY3	А	2000	-	-	0/27/44/44	0/3/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	2000	ZY3	O2-S	2.55	1.46	1.43
2	А	2000	ZY3	C11-C12	2.45	1.53	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	2000	ZY3	C11-C12-C7	4.58	124.49	118.33
2	А	2000	ZY3	C11-C10-C9	-3.29	109.84	114.42
2	А	2000	ZY3	C2-N1-C3	-3.15	116.68	123.21
2	А	2000	ZY3	C22-C23-N4	-2.86	108.05	111.97
2	А	2000	ZY3	C24-N4-C23	2.73	124.21	113.60
2	А	2000	ZY3	C5-C6-C7	2.12	122.80	118.61

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	2502	GOL	O1-C1-C2-O2
3	А	2502	GOL	O1-C1-C2-C3
3	А	2502	GOL	C1-C2-C3-O3

Continued on next page...



Mol	Chain	Res	Type	Atoms
3	А	2501	GOL	C1-C2-C3-O3
3	А	2500	GOL	O1-C1-C2-C3
3	А	2503	GOL	O1-C1-C2-C3
3	А	2500	GOL	O1-C1-C2-O2
3	А	2503	GOL	C1-C2-C3-O3
3	А	2502	GOL	O2-C2-C3-O3
3	А	2501	GOL	O2-C2-C3-O3
3	А	2503	GOL	O1-C1-C2-O2
3	А	2501	GOL	O1-C1-C2-O2
3	А	2503	GOL	O2-C2-C3-O3
3	А	2501	GOL	O1-C1-C2-C3

Continued from previous page...

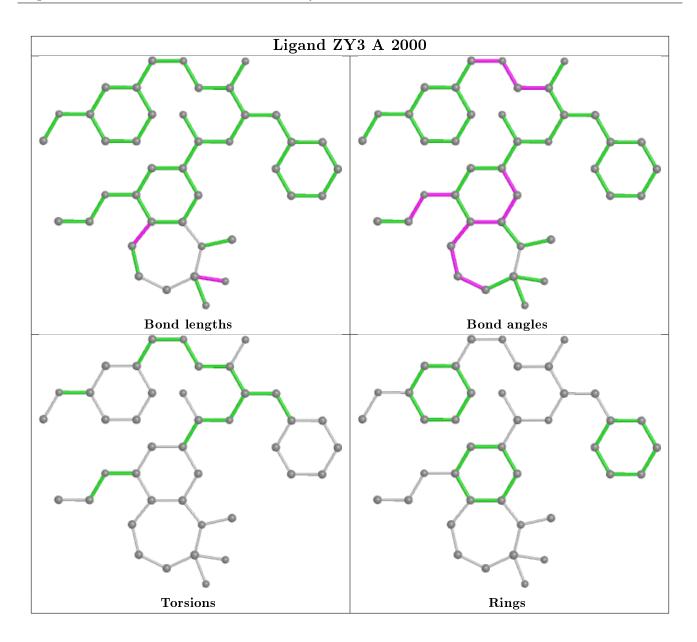
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	2501	GOL	6	0
3	А	2500	GOL	3	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.





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^{th} 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	ysed $\langle RSRZ \rangle = \#RSRZ \rangle 2$		$OWAB(Å^2)$	Q<0.9	
1	А	375/392~(95%)	-0.16	6 (1%) 72 7	5	9,21,35,47	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	447	ILE	4.9
1	А	446	ASN	3.3
1	А	206	HIS	3.2
1	А	229	ALA	2.6
1	А	438	LEU	2.4
1	А	440	MET	2.4

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^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	GOL	А	2503	6/6	0.83	0.43	54, 55, 57, 58	0

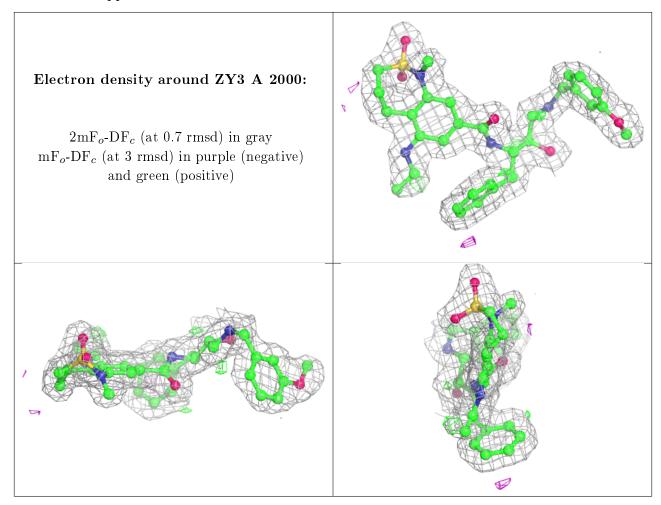
Continued on next page...



Continucu from previous page									
Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	${f B} ext{-factors}({ m \AA}^2)$	$Q{<}0.9$	
3	GOL	A	2502	6/6	0.88	0.18	$38,\!46,\!46,\!48$	0	
3	GOL	А	2501	6/6	0.89	0.20	$31,\!39,\!41,\!46$	0	
3	GOL	А	2500	6/6	0.90	0.17	$30,\!37,\!38,\!43$	0	
2	ZY3	А	2000	41/41	0.97	0.10	$8,\!14,\!20,\!22$	0	

Continued from previous page...

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.



6.5 Other polymers (i)

There are no such residues in this entry.

