wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 02:19 PM EDT

PDB ID	:	1BQM
Title	:	HIV-1 RT/HBY 097
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Deposited on	:	1998-08-17
Resolution	:	3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

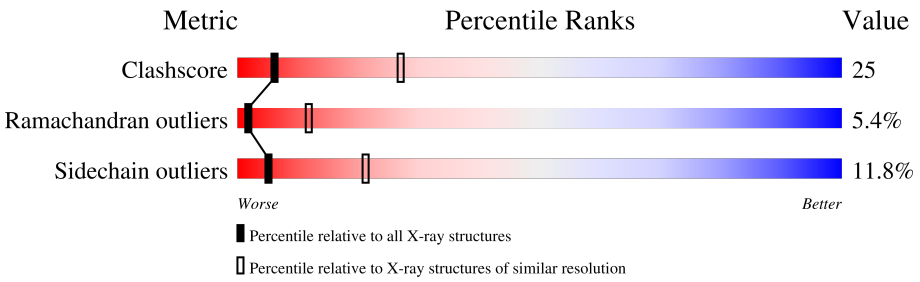
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	51% 42% 6%
2	B	430	47% 46% 6% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HBY	A	557	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7799 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4338	2804	719	808	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

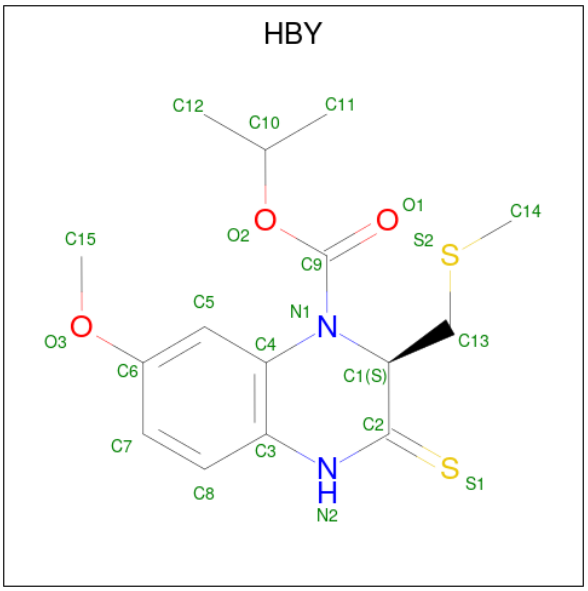
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	430	3439	2240	567	627	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is (S)-4-ISOPROPOXYCARBONYL-6-METHOXY-3-METHYLTHIOMETHYL-3,4-DIHYDROQUINOXALIN-2(1H)-THIONE (three-letter code: HBY) (formula: $C_{15}H_{20}N_2O_3S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	22	15	2	3	2	0	0

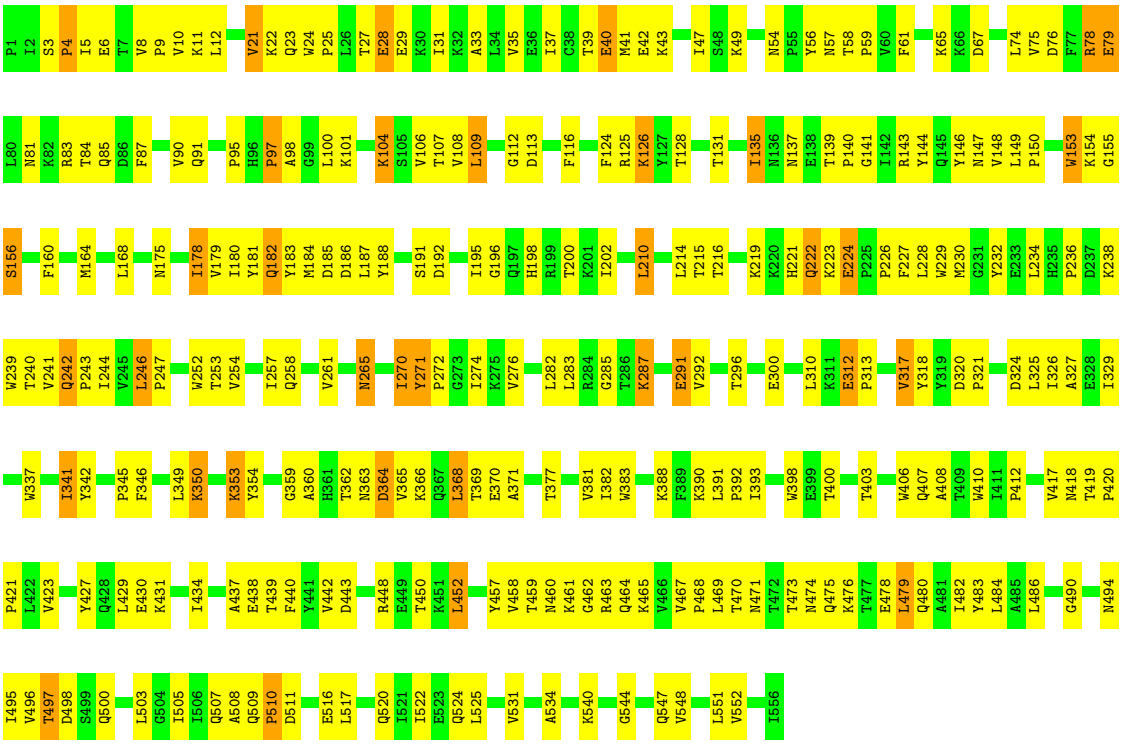
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

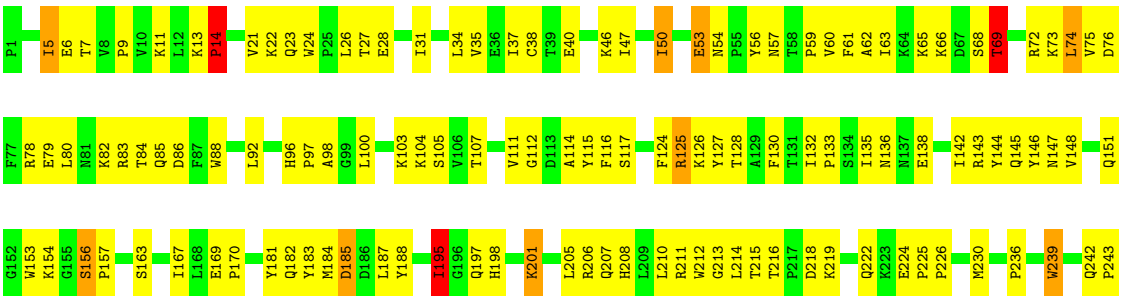
• Molecule 1: REVERSE TRANSCRIPTASE

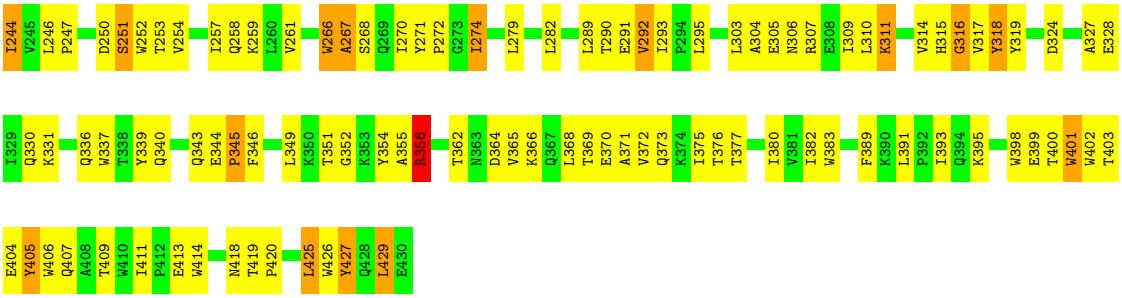
Chain A: 51% 42% 6%



• Molecule 2: REVERSE TRANSCRIPTASE

Chain B: 47% 46% 6%




I244 V245 L246 P247
D250 S251 W252 T253 V254
I257 Q258 K259 L260 V261
W266 A267 S268 Q269 I270 Y271 P272 G273 I274
L279
L282
L289 T290 E291 V292 I293 P294 L295
L303 A304 E305 N306 R307 E308 I309 L310 K311
V314 H315 G316 V317 Y318 Y319
D324
A327 E328
I329 Q330 K331
Q336 W337 T338 Y339 Q340
Q343 E344 P345 F346
L349 K350 T351 G352 K353 Y354 A355 R356
T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377
I380 V381 I382 W383
F389 K390 L391 P392 I393 Q394 K395
W398 E399 T400 W401 W402 T403
E404 Y405 W406 Q407 A408 T409 W410 I411 P412 E413 W414
N418 T419 P420
L425 W426 Y427 Q428 L429 E430

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.20Å 69.40Å 104.60Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	99.1 (10.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.258 , 0.362	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7799	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

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: HBY

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	0.50	0/4451	0.77	0/6070
2	B	0.54	0/3538	0.84	1/4821 (0.0%)
All	All	0.52	0/7989	0.80	1/10891 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	TRP	N-CA-C	5.35	125.44	111.00

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	4338	0	4229	213	0
2	B	3439	0	3390	172	0
3	A	22	0	20	25	0
All	All	7799	0	7639	379	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 25.

The worst 5 of 379 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)
2:B:26:LEU:HD12	2:B:133:PRO:HG3	1.41	1.03
1:A:327:ALA:HB2	1:A:341:ILE:HG23	1.46	0.97
1:A:242:GLN:HB3	1:A:243:PRO:HD3	1.50	0.92
1:A:234:LEU:HB3	3:A:557:HBY:H153	1.53	0.90
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.55	0.89

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	554/556 (100%)	453 (82%)	75 (14%)	26 (5%)	2 14
2	B	428/430 (100%)	342 (80%)	59 (14%)	27 (6%)	1 8
All	All	982/986 (100%)	795 (81%)	134 (14%)	53 (5%)	2 12

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	67	ASP
1	A	104	LYS
1	A	195	ILE
1	A	222	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	450/496 (91%)	390 (87%)	60 (13%)	4 16
2	B	363/392 (93%)	327 (90%)	36 (10%)	8 29
All	All	813/888 (92%)	717 (88%)	96 (12%)	5 21

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	516	GLU
2	B	163	SER
1	A	547	GLN
2	B	60	VAL
2	B	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	182	GLN
2	B	258	GLN
2	B	208	HIS
2	B	330	GLN
1	A	265	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	HBY	A	557	-	23,23,23	7.37	19 (82%)	24,32,32	2.05	6 (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	HBY	A	557	-	-	5/13/29/29	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	557	HBY	C1-C2	17.63	1.67	1.50
3	A	557	HBY	C9-N1	13.64	1.57	1.37
3	A	557	HBY	C3-C4	11.96	1.54	1.40
3	A	557	HBY	C2-S1	10.42	1.82	1.66
3	A	557	HBY	C1-N1	8.66	1.58	1.47

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	557	HBY	O2-C9-N1	6.23	118.10	110.81
3	A	557	HBY	C3-N2-C2	-4.84	120.51	124.74
3	A	557	HBY	O1-C9-N1	-2.86	119.29	124.09
3	A	557	HBY	O2-C10-C12	2.45	113.65	107.14
3	A	557	HBY	C14-S2-C13	-2.44	96.81	101.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	557	HBY	C2-C1-C13-S2
3	A	557	HBY	N1-C1-C13-S2
3	A	557	HBY	N1-C9-O2-C10
3	A	557	HBY	O1-C9-O2-C10
3	A	557	HBY	C11-C10-O2-C9

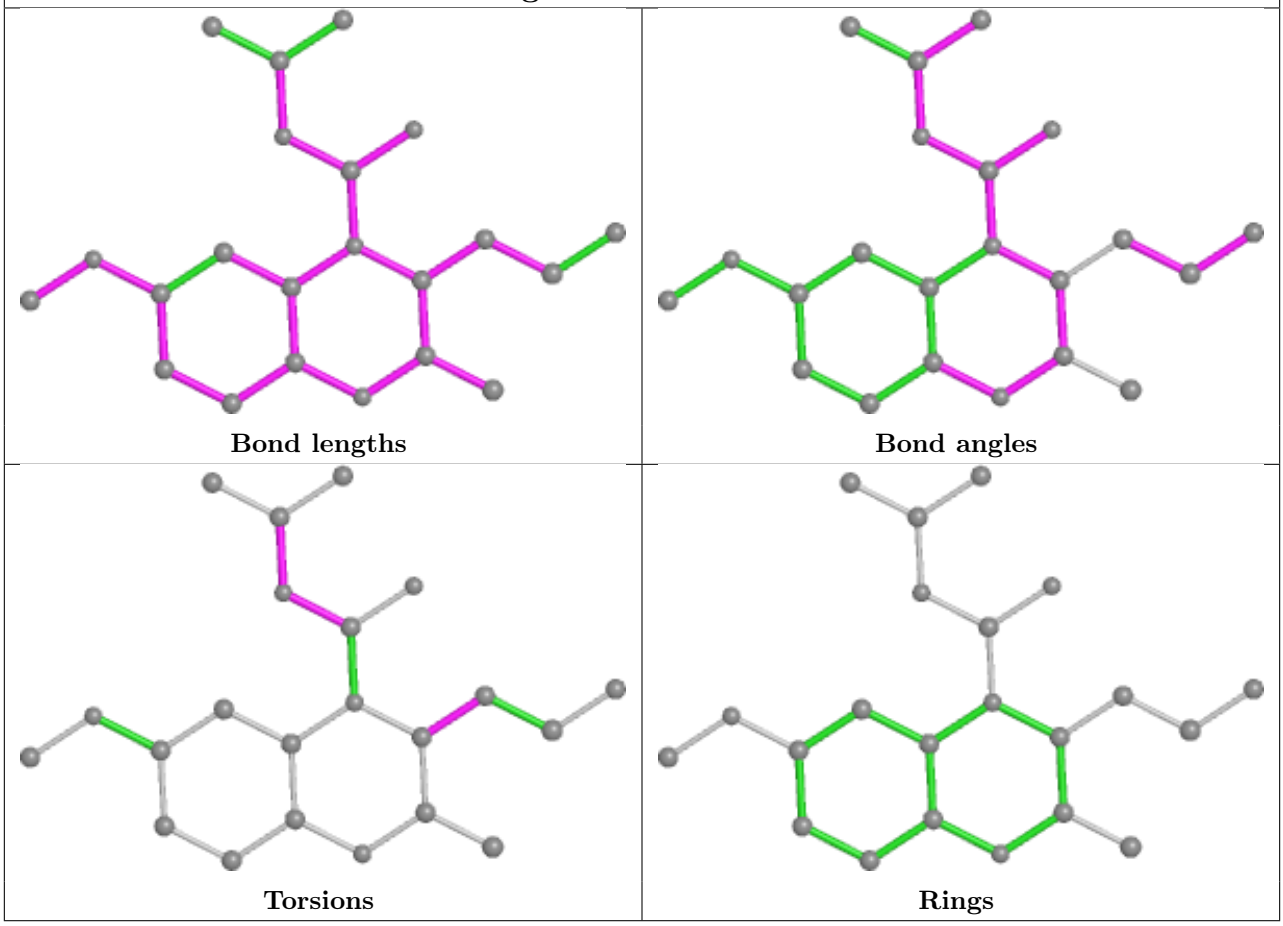
There are no ring outliers.

1 monomer is involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	HBY	25	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HBY A 557



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.