

Full wwPDB X-ray Structure Validation 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 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:

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: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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	Quali	ty of chain	
1	А	556	51%	42%	6%
2	В	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	А	557	-	-	Х	-



1BQM

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
1	А	556	Total 4338	C 2804	N 710	0 808	${ m S}_7$	0	0	0
			4000	2004	119	000	1			

There is a discrepancy between the modelled and reference sequences:

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

• Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	430	Total 3439	C 2240	N 567	O 627	${ m S}{ m 5}$	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

• Molecule 3 is (S)-4-ISOPROPOXYCARBONYL-6-METHOXY-3-METHYLTHIOMET HYL-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		
3	А	1	Total 22	C 15	N 2	O 3	${ m S} { m 2}$	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.







E404 1329 1244 V406 X331 1244 V406 X331 1246 V406 X331 1246 V406 X331 1246 V410 T336 X345 V410 T336 X355 V411 X339 X256 V413 T336 X256 V414 X349 X255 V416 X360 X256 V426 X360 X266 V426 X366 X266 V426 X366 X266 V427 X366 X266 V428 X366 X266 V428 X366 X266 V428 X366 X266 V428 X366 X266 V438 X366 X266



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	225.20Å 69.40Å 104.60Å	Depositor
a, b, c, α , β , γ	90.00° 106.40° 90.00°	Depositor
Resolution (Å)	10.00 - 3.10	Depositor
% Data completeness	99.1 (10.00-3.10)	Depositor
(in resolution range)	55.1 (10.00 0.10)	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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.50	0/4451	0.77	0/6070	
2	В	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	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	В	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	А	4338	0	4229	213	0
2	В	3439	0	3390	172	0
3	А	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.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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
2:B:38:CYS:HB3	2:B:144:TYR:HE2	1.36	0.88
2:B:210:LEU:HD11	2:B:216:THR:HG23	1.56	0.87
2:B:183:TYR:CE2	2:B:380:ILE:HD12	2.10	0.87
1:A:227:PHE:HD2	3:A:557:HBY:H151	1.40	0.86
1:A:188:TYR:O	3:A:557:HBY:C14	2.24	0.85
1:A:9:PRO:HG2	2:B:53:GLU:HG2	1.59	0.84
2:B:26:LEU:HD12	2:B:133:PRO:CG	2.08	0.83
1:A:98:ALA:HB2	1:A:350:LYS:HG3	1.62	0.82
1:A:419:THR:HG22	1:A:421:PRO:HD2	1.62	0.82
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.15	0.81
2:B:63:ILE:HD11	2:B:74:LEU:HD22	1.59	0.81
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.15	0.81
1:A:240:THR:HG22	1:A:241:VAL:H	1.43	0.81
2:B:339:TYR:CD2	2:B:375:ILE:HD12	2.15	0.81
2:B:305:GLU:O	2:B:309:ILE:HG13	1.79	0.80
1:A:257:ILE:O	1:A:261:VAL:HG23	1.81	0.80
1:A:188:TYR:CE2	3:A:557:HBY:H121	2.18	0.78
2:B:368:LEU:O	2:B:372:VAL:HG23	1.84	0.78
1:A:100:LEU:HD11	3:A:557:HBY:H111	1.66	0.78
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.48	0.78
1:A:430:GLU:HG2	1:A:531:VAL:O	1.83	0.77
1:A:476:LYS:HG3	1:A:517:LEU:HD22	1.64	0.77
1:A:417:VAL:HG12	1:A:418:ASN:H	1.50	0.77
2:B:369:THR:HG23	2:B:406:TRP:HE3	1.49	0.76
1:A:483:TYR:HE1	1:A:524:GLN:HE21	1.33	0.75
2:B:13:LYS:HG2	2:B:14:PRO:HD2	1.68	0.75
1:A:12:LEU:HD23	1:A:84:THR:HA	1.69	0.74
2:B:425:LEU:HD23	2:B:426:TRP:H	1.52	0.74
1:A:459:THR:OG1	1:A:463:ARG:HB3	1.86	0.73
2:B:27:THR:O	2:B:31:ILE:HG13	1.88	0.73
2:B:197:GLN:O	2:B:201:LYS:HE2	1.88	0.73
2:B:319:TYR:HD1	2:B:343:GLN:HE22	1.37	0.72
1:A:100:LEU:HD13	3:A:557:HBY:C4	2.19	0.72
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.70	0.72
1:A:100:LEU:HD13	3:A:557:HBY:N1	2.04	0.72

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:101:LYS:HE2	1:A:321:PRO:HD3	1.69	0.72
1:A:326:ILE:HG22	1:A:342:TYR:O	1.90	0.71
2:B:368:LEU:HD21	2:B:391:LEU:HD22	1.71	0.71
1:A:382:ILE:O	2:B:136:ASN:HB2	1.90	0.71
2:B:125:ARG:HG2	2:B:146:TYR:O	1.90	0.71
1:A:98:ALA:CB	1:A:350:LYS:HG3	2.21	0.71
2:B:13:LYS:HD2	2:B:83:ARG:O	1.90	0.70
2:B:27:THR:HG22	2:B:28:GLU:N	2.06	0.70
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.21	0.70
1:A:420:PRO:HG2	1:A:421:PRO:HD3	1.74	0.70
1:A:21:VAL:HG12	1:A:22:LYS:H	1.56	0.69
1:A:483:TYR:HE1	1:A:524:GLN:NE2	1.91	0.69
2:B:310:LEU:O	2:B:311:LYS:HD2	1.92	0.69
1:A:366:LYS:O	1:A:370:GLU:HG3	1.92	0.69
2:B:5:ILE:HG22	2:B:6:GLU:H	1.58	0.69
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.07	0.69
1:A:79:GLU:O	1:A:83:ARG:HD2	1.93	0.68
1:A:439:THR:H	1:A:460:ASN:ND2	1.90	0.68
2:B:351:THR:HG21	2:B:429:LEU:HB3	1.74	0.68
1:A:188:TYR:O	3:A:557:HBY:H141	1.94	0.68
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.75	0.68
1:A:242:GLN:CB	1:A:243:PRO:HD3	2.24	0.68
1:A:227:PHE:CD2	3:A:557:HBY:H151	2.28	0.68
1:A:229:TRP:NE1	3:A:557:HBY:H113	2.09	0.68
2:B:13:LYS:CG	2:B:14:PRO:HD2	2.23	0.67
1:A:382:ILE:HG23	2:B:136:ASN:OD1	1.94	0.67
1:A:31:ILE:O	1:A:35:VAL:HG23	1.95	0.67
1:A:188:TYR:O	3:A:557:HBY:H143	1.94	0.67
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.59	0.67
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.60	0.67
1:A:229:TRP:CD2	3:A:557:HBY:H122	2.29	0.66
1:A:240:THR:HG22	1:A:241:VAL:N	2.11	0.66
1:A:253:THR:HA	1:A:292:VAL:HA	1.78	0.66
2:B:395:LYS:HG2	2:B:399:GLU:OE2	1.96	0.66
2:B:79:GLU:O	2:B:83:ARG:HG2	1.96	0.66
2:B:31:ILE:O	2:B:35:VAL:HG23	1.97	0.65
1:A:496:VAL:HA	1:A:534:ALA:HB3	1.78	0.64
2:B:303:LEU:O	2:B:307:ARG:HB2	1.98	0.64
1:A:100:LEU:HD22	3:A:557:HBY:H1	1.79	0.64
1:A:377:THR:O	1:A:381:VAL:HG23	1.98	0.64
2:B:21:VAL:HG12	2:B:22:LYS:H	1.63	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:149:LEU:HD13	1:A:156:SER:HA	1.81	0.63
1:A:282:LEU:H	1:A:282:LEU:HD23	1.64	0.63
2:B:405:TYR:CD1	2:B:405:TYR:N	2.66	0.63
1:A:8:VAL:HG13	1:A:9:PRO:HD2	1.79	0.63
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.80	0.63
2:B:224:GLU:HG2	2:B:225:PRO:HD2	1.80	0.63
1:A:417:VAL:HG12	1:A:418:ASN:N	2.14	0.63
2:B:61:PHE:CZ	2:B:402:TRP:CZ2	2.87	0.63
1:A:479:LEU:HB3	1:A:517:LEU:HD21	1.81	0.62
2:B:405:TYR:HD1	2:B:405:TYR:H	1.46	0.62
1:A:33:ALA:O	1:A:37:ILE:HD13	1.99	0.62
1:A:318:TYR:CE2	3:A:557:HBY:H8	2.34	0.62
2:B:183:TYR:CD2	2:B:380:ILE:HD12	2.33	0.62
2:B:183:TYR:HE2	2:B:380:ILE:HD12	1.63	0.62
1:A:191:SER:OG	1:A:198:HIS:CD2	2.53	0.62
2:B:339:TYR:CG	2:B:375:ILE:HD12	2.34	0.62
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.65	0.62
1:A:10:VAL:HG12	1:A:124:PHE:CE2	2.35	0.61
2:B:54:ASN:OD1	2:B:56:TYR:HD1	1.81	0.61
2:B:167:ILE:O	2:B:208:HIS:HE1	1.83	0.61
2:B:304:ALA:HA	2:B:307:ARG:HB3	1.82	0.61
1:A:108:VAL:HA	1:A:187:LEU:O	2.00	0.61
2:B:63:ILE:CD1	2:B:74:LEU:HD22	2.31	0.61
2:B:61:PHE:CZ	2:B:402:TRP:HZ2	2.20	0.60
1:A:438:GLU:HG3	1:A:460:ASN:ND2	2.16	0.60
2:B:181:TYR:CD1	2:B:182:GLN:N	2.69	0.60
2:B:279:LEU:O	2:B:282:LEU:HB3	2.01	0.60
2:B:270:ILE:O	2:B:272:PRO:HD3	2.02	0.60
1:A:116:PHE:O	1:A:148:VAL:HG11	2.01	0.60
1:A:544:GLY:O	1:A:548:VAL:HG23	2.02	0.59
1:A:551:LEU:HD12	1:A:552:VAL:HG13	1.84	0.59
1:A:188:TYR:CD2	3:A:557:HBY:H121	2.36	0.59
1:A:198:HIS:O	1:A:202:ILE:HG12	2.02	0.59
2:B:207:GLN:O	2:B:211:ARG:HG3	2.03	0.59
1:A:224:GLU:HB2	1:A:226:PRO:HD2	1.85	0.59
1:A:369:THR:OG1	1:A:398:TRP:CZ3	2.56	0.59
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.49	0.59
1:A:49:LYS:HA	1:A:144:TYR:HA	1.84	0.59
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.84	0.58
1:A:108:VAL:O	1:A:223:LYS:HG3	2.02	0.58
2:B:291:GLU:O	2:B:293:ILE:HG23	2.04	0.58



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Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:96:HIS:HD2	2:B:181:TYR:CE2	2.22	0.58
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.29	0.57
2:B:27:THR:CG2	2:B:28:GLU:N	2.68	0.57
2:B:21:VAL:HG12	2:B:22:LYS:N	2.20	0.57
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.86	0.57
2:B:181:TYR:HD1	2:B:182:GLN:N	2.02	0.57
1:A:101:LYS:NZ	1:A:321:PRO:HG3	2.20	0.56
1:A:141:GLY:O	1:A:143:ARG:HG2	2.05	0.56
1:A:393:ILE:HD11	1:A:398:TRP:HB2	1.87	0.56
1:A:438:GLU:HB3	1:A:440:PHE:HE1	1.70	0.56
1:A:270:ILE:HD12	1:A:270:ILE:H	1.69	0.56
2:B:7:THR:O	2:B:9:PRO:HD3	2.05	0.56
2:B:63:ILE:HD13	2:B:406:TRP:O	2.05	0.56
2:B:345:PRO:O	2:B:346:PHE:HB2	2.04	0.56
1:A:168:LEU:HD22	1:A:180:ILE:CD1	2.36	0.56
1:A:95:PRO:HD2	1:A:229:TRP:HZ2	1.71	0.56
1:A:350:LYS:NZ	1:A:350:LYS:HB3	2.21	0.56
1:A:3:SER:OG	1:A:5:ILE:HG22	2.06	0.55
1:A:131:THR:OG1	1:A:143:ARG:HB3	2.06	0.55
1:A:261:VAL:HG13	1:A:276:VAL:HG12	1.88	0.55
2:B:154:LYS:HG3	2:B:184:MET:SD	2.47	0.55
1:A:475:GLN:HA	1:A:478:GLU:OE1	2.07	0.55
2:B:266:TRP:C	2:B:268:SER:H	2.08	0.55
1:A:229:TRP:HB3	1:A:234:LEU:HD12	1.89	0.55
2:B:239:TRP:NE1	2:B:382:ILE:HD11	2.22	0.54
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.42	0.54
1:A:196:GLY:O	1:A:200:THR:HG23	2.06	0.54
2:B:112:GLY:HA3	2:B:185:ASP:HB3	1.87	0.54
2:B:183:TYR:CD2	2:B:380:ILE:HG23	2.43	0.54
2:B:239:TRP:HE1	2:B:382:ILE:HD11	1.73	0.54
1:A:350:LYS:HB3	1:A:350:LYS:HZ2	1.72	0.54
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.38	0.53
2:B:181:TYR:HD1	2:B:182:GLN:H	1.56	0.53
1:A:139:THR:N	1:A:140:PRO:HD3	2.23	0.53
2:B:37:ILE:HG22	2:B:38:CYS:N	2.23	0.53
1:A:100:LEU:HD22	3:A:557:HBY:C2	2.39	0.53
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.74	0.53
2:B:151:GLN:HG2	2:B:185:ASP:OD2	2.09	0.53
1:A:59:PRO:HG3	1:A:78:ARG:HH21	1.74	0.53
1:A:100:LEU:HD22	3:A:557:HBY:C1	2.39	0.52
2:B:126:LYS:HE3	2:B:127:TYR:CE1	2.44	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:293:ILE:HG13	2:B:293:ILE:O	2.08	0.52
2:B:253:THR:HG22	2:B:292:VAL:HA	1.90	0.52
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.44	0.52
2:B:373:GLN:HE22	2:B:407:GLN:N	2.06	0.52
3:A:557:HBY:O2	3:A:557:HBY:H5	2.10	0.52
1:A:125:ARG:HH11	1:A:147:ASN:HD22	1.58	0.52
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.91	0.52
2:B:225:PRO:N	2:B:226:PRO:HD2	2.23	0.52
2:B:195:ILE:HD13	2:B:195:ILE:H	1.75	0.51
1:A:41:MET:HB3	1:A:47:ILE:HD11	1.93	0.51
1:A:520:GLN:O	1:A:524:GLN:HG2	2.10	0.51
2:B:27:THR:HG22	2:B:28:GLU:H	1.76	0.51
2:B:124:PHE:CE1	2:B:127:TYR:HD2	2.29	0.51
2:B:340:GLN:NE2	2:B:429:LEU:HA	2.25	0.51
1:A:56:TYR:N	1:A:56:TYR:CD1	2.78	0.51
1:A:393:ILE:HD13	1:A:398:TRP:HE3	1.76	0.51
1:A:210:LEU:HD22	1:A:215:THR:HA	1.93	0.51
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.41	0.51
1:A:354:TYR:CD2	1:A:371:ALA:HB2	2.46	0.51
2:B:356:ARG:HA	2:B:356:ARG:NE	2.26	0.51
2:B:63:ILE:HD12	2:B:74:LEU:HD13	1.93	0.50
2:B:251:SER:HB2	2:B:295:LEU:HD21	1.93	0.50
1:A:329:ILE:HD12	1:A:391:LEU:HD21	1.93	0.50
1:A:508:ALA:C	1:A:509:GLN:HG2	2.30	0.50
1:A:11:LYS:N	1:A:85:GLN:OE1	2.44	0.50
1:A:106:VAL:HG12	1:A:107:THR:N	2.27	0.50
1:A:508:ALA:O	1:A:509:GLN:HG2	2.12	0.50
2:B:257:ILE:O	2:B:261:VAL:HG23	2.11	0.50
1:A:10:VAL:CG1	1:A:124:PHE:CE2	2.94	0.50
1:A:23:GLN:O	1:A:25:PRO:HD3	2.11	0.50
1:A:108:VAL:HG22	1:A:188:TYR:CD1	2.46	0.50
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.94	0.50
2:B:336:GLN:HA	2:B:355:ALA:HA	1.93	0.50
1:A:392:PRO:O	1:A:423:VAL:HG23	2.12	0.50
1:A:182:GLN:HE21	1:A:183:TYR:N	2.11	0.49
1:A:191:SER:OG	1:A:198:HIS:HD2	1.95	0.49
1:A:56:TYR:O	1:A:57:ASN:HB2	2.11	0.49
2:B:369:THR:HG23	2:B:406:TRP:CE3	2.38	0.49
1:A:8:VAL:CG1	1:A:9:PRO:HD2	2.43	0.49
2:B:34:LEU:HD21	2:B:61:PHE:O	2.11	0.49
2:B:65:LYS:HB2	2:B:72:ARG:HG3	1.93	0.48



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:182:GLN:O	1:A:182:GLN:HG3	2.12	0.48
2:B:156:SER:H	2:B:157:PRO:HD2	1.78	0.48
1:A:470:THR:O	1:A:471:ASN:HB2	2.13	0.48
2:B:210:LEU:O	2:B:213:GLY:O	2.31	0.48
1:A:160:PHE:CE2	1:A:182:GLN:OE1	2.67	0.48
2:B:310:LEU:C	2:B:311:LYS:HD2	2.33	0.48
2:B:349:LEU:HD22	2:B:383:TRP:HZ2	1.79	0.48
2:B:371:ALA:O	2:B:375:ILE:HG12	2.13	0.48
2:B:239:TRP:CD1	2:B:382:ILE:HD11	2.48	0.48
1:A:229:TRP:CE2	3:A:557:HBY:H122	2.49	0.48
1:A:258:GLN:HE21	1:A:283:LEU:HD21	1.77	0.48
1:A:100:LEU:HB3	3:A:557:HBY:N2	2.29	0.48
2:B:5:ILE:HG22	2:B:6:GLU:N	2.27	0.48
2:B:135:ILE:HD12	2:B:135:ILE:H	1.78	0.48
1:A:186:ASP:HB3	1:A:188:TYR:HE1	1.79	0.48
1:A:224:GLU:OE1	1:A:226:PRO:HG2	2.13	0.48
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.49	0.48
2:B:344:GLU:HA	2:B:345:PRO:HD2	1.61	0.48
2:B:206:ARG:HH12	2:B:219:LYS:HA	1.79	0.47
1:A:39:THR:HG22	1:A:39:THR:O	2.14	0.47
1:A:483:TYR:CE1	1:A:524:GLN:NE2	2.76	0.47
2:B:27:THR:CG2	2:B:28:GLU:H	2.26	0.47
1:A:410:TRP:HB2	2:B:365:VAL:HG23	1.96	0.47
1:A:87:PHE:CE2	1:A:155:GLY:HA3	2.49	0.47
1:A:291:GLU:HG3	1:A:291:GLU:O	2.13	0.47
1:A:427:TYR:CE2	1:A:525:LEU:HD13	2.49	0.47
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.78	0.47
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.44	0.47
2:B:107:THR:OG1	2:B:198:HIS:HE1	1.98	0.47
1:A:420:PRO:HG2	1:A:421:PRO:CD	2.44	0.47
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.76	0.47
2:B:267:ALA:O	2:B:271:TYR:HB2	2.14	0.47
1:A:282:LEU:HD13	1:A:296:THR:HG23	1.98	0.46
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.73	0.46
2:B:103:LYS:O	2:B:105:SER:N	2.48	0.46
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.15	0.46
2:B:100:LEU:HD22	2:B:181:TYR:HB2	1.96	0.46
2:B:244:ILE:HG22	2:B:244:ILE:O	2.14	0.46
1:A:178:ILE:HA	1:A:191:SER:HB3	1.97	0.46
1:A:407:GLN:HG3	2:B:393:ILE:HA	1.97	0.46
2:B:210:LEU:CD1	2:B:216:THR:HG23	2.37	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:326:ILE:HD11	1:A:390:LYS:HG2	1.97	0.46
2:B:50:ILE:HG12	2:B:145:GLN:HB2	1.98	0.46
2:B:31:ILE:O	2:B:31:ILE:HG22	2.16	0.46
2:B:214:LEU:HD12	2:B:214:LEU:HA	1.66	0.46
2:B:247:PRO:HB2	2:B:250:ASP:CB	2.46	0.46
2:B:402:TRP:O	2:B:404:GLU:N	2.49	0.46
2:B:425:LEU:HD23	2:B:427:TYR:H	1.81	0.46
1:A:40:GLU:HG2	1:A:43:LYS:HD2	1.97	0.46
1:A:312:GLU:HA	1:A:313:PRO:HD2	1.65	0.45
2:B:47:ILE:HD12	2:B:130:PHE:HZ	1.81	0.45
2:B:400:THR:HG22	2:B:401:TRP:CD1	2.50	0.45
1:A:112:GLY:HA2	1:A:185:ASP:HB3	1.98	0.45
2:B:78:ARG:HD3	2:B:411:ILE:O	2.15	0.45
2:B:254:VAL:HG23	2:B:291:GLU:O	2.16	0.45
2:B:398:TRP:O	2:B:402:TRP:HD1	1.99	0.45
1:A:227:PHE:HD2	3:A:557:HBY:C15	2.21	0.45
1:A:329:ILE:CD1	1:A:391:LEU:HD21	2.47	0.45
1:A:443:ASP:HB2	1:A:548:VAL:CG1	2.47	0.45
2:B:115:TYR:C	2:B:117:SER:H	2.20	0.45
2:B:111:VAL:HG12	2:B:111:VAL:O	2.17	0.45
1:A:109:LEU:HD23	1:A:216:THR:CG2	2.47	0.45
1:A:500:GLN:O	1:A:503:LEU:HB3	2.16	0.45
2:B:354:TYR:CE2	2:B:371:ALA:HB2	2.52	0.45
1:A:175:ASN:O	1:A:178:ILE:HG22	2.17	0.45
1:A:406:TRP:O	2:B:331:LYS:NZ	2.50	0.45
2:B:46:LYS:O	2:B:147:ASN:HB2	2.16	0.45
2:B:315:HIS:O	2:B:316:GLY:C	2.55	0.45
2:B:365:VAL:HG12	2:B:365:VAL:O	2.17	0.45
1:A:90:VAL:HG23	1:A:91:GLN:N	2.32	0.44
1:A:180:ILE:HG22	1:A:181:TYR:N	2.32	0.44
1:A:285:GLY:C	1:A:287:LYS:H	2.20	0.44
2:B:419:THR:HA	2:B:420:PRO:HD3	1.80	0.44
1:A:100:LEU:HD13	3:A:557:HBY:C3	2.47	0.44
2:B:339:TYR:CD1	2:B:352:GLY:O	2.71	0.44
1:A:452:LEU:HD12	1:A:452:LEU:O	2.18	0.44
2:B:376:THR:O	2:B:380:ILE:HG12	2.17	0.44
2:B:400:THR:CG2	2:B:401:TRP:CD1	3.01	0.44
1:A:443:ASP:HB2	1:A:548:VAL:HG12	1.99	0.44
2:B:274:ILE:HG12	2:B:306:ASN:OD1	2.18	0.44
2:B:314:VAL:HG23	2:B:315:HIS:H	1.82	0.44
1:A:240:THR:CG2	1:A:241:VAL:H	2.21	0.44



	r ar Fagana	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:337:TRP:CZ3	1:A:368:LEU:HD12	2.52	0.44	
2:B:114:ALA:CB	2:B:215:THR:HG22	2.48	0.44	
1:A:168:LEU:HD22	1:A:180:ILE:HD13	2.00	0.44	
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.99	0.44	
2:B:132:ILE:HB	2:B:142:ILE:HB	2.00	0.44	
1:A:254:VAL:HG23	1:A:291:GLU:HG3	2.00	0.43	
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.35	0.43	
2:B:327:ALA:O	2:B:389:PHE:HA	2.18	0.43	
1:A:54:ASN:HD22	1:A:143:ARG:HH21	1.65	0.43	
1:A:59:PRO:O	1:A:75:VAL:HG13	2.18	0.43	
1:A:246:LEU:O	1:A:246:LEU:HD12	2.18	0.43	
1:A:365:VAL:O	1:A:368:LEU:HB3	2.17	0.43	
1:A:393:ILE:CD1	1:A:398:TRP:HB2	2.48	0.43	
2:B:80:LEU:O	2:B:84:THR:N	2.52	0.43	
1:A:482:ILE:HG23	1:A:495:ILE:HG21	2.00	0.43	
1:A:178:ILE:O	1:A:178:ILE:HG23	2.19	0.43	
2:B:111:VAL:HG21	2:B:187:LEU:HD22	2.00	0.43	
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.64	0.43	
1:A:497:THR:HG22	1:A:498:ASP:N	2.34	0.43	
2:B:355:ALA:O	2:B:356:ARG:HB2	2.18	0.43	
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.74	0.43	
1:A:511:ASP:O	1:A:522:ILE:HD13	2.19	0.43	
1:A:229:TRP:CE3	1:A:230:MET:HG2	2.54	0.43	
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.53	0.43	
2:B:210:LEU:HD12	2:B:210:LEU:HA	1.71	0.43	
1:A:390:LYS:HA	1:A:390:LYS:HD3	1.72	0.43	
1:A:317:VAL:HG12	1:A:349:LEU:HA	2.00	0.42	
2:B:85:GLN:HA	2:B:88:TRP:HB2	2.01	0.42	
1:A:246:LEU:H	1:A:246:LEU:HG	1.52	0.42	
1:A:363:ASN:OD1	1:A:364:ASP:N	2.53	0.42	
1:A:437:ALA:HB3	1:A:494:ASN:ND2	2.33	0.42	
1:A:438:GLU:HA	1:A:460:ASN:HD21	1.84	0.42	
1:A:509:GLN:N	1:A:510:PRO:HD3	2.33	0.42	
2:B:259:LYS:HD3	2:B:426:TRP:HH2	1.84	0.42	
2:B:266:TRP:C	2:B:268:SER:N	2.73	0.42	
2:B:274:ILE:HG23	2:B:306:ASN:HD21	1.84	0.42	
2:B:337:TRP:HB2	2:B:354:TYR:HB3	2.02	0.42	
1:A:222:GLN:O	1:A:223:LYS:HG2	2.20	0.42	
1:A:229:TRP:CD1	1:A:234:LEU:HD11	2.54	0.42	
1:A:458:VAL:HG22	1:A:464:GLN:HG2	2.00	0.42	
2:B:38:CYS:SG	2:B:73:LYS:NZ	2.85	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:265:ASN:HD21	1:A:353:LYS:NZ	2.18	0.42
2:B:366:LYS:O	2:B:370:GLU:HG3	2.20	0.42
1:A:234:LEU:CB	3:A:557:HBY:H153	2.37	0.42
1:A:5:ILE:HG13	1:A:6:GLU:N	2.35	0.42
1:A:160:PHE:HE2	1:A:182:GLN:OE1	2.03	0.42
2:B:115:TYR:N	2:B:115:TYR:CD1	2.85	0.42
2:B:242:GLN:N	2:B:243:PRO:HD3	2.35	0.42
1:A:467:VAL:HA	1:A:468:PRO:HD2	1.81	0.42
1:A:482:ILE:O	1:A:486:LEU:N	2.52	0.42
2:B:316:GLY:O	2:B:318:TYR:N	2.52	0.42
2:B:368:LEU:HG	2:B:398:TRP:CZ3	2.55	0.42
1:A:271:TYR:HA	1:A:272:PRO:HD2	1.79	0.42
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.55	0.42
2:B:368:LEU:HD23	2:B:398:TRP:CZ3	2.55	0.42
1:A:239:TRP:O	1:A:240:THR:OG1	2.34	0.41
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.49	0.41
2:B:73:LYS:HG2	2:B:74:LEU:N	2.34	0.41
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.85	0.41
1:A:369:THR:O	1:A:369:THR:HG22	2.19	0.41
2:B:65:LYS:HB2	2:B:72:ARG:CG	2.50	0.41
1:A:221:HIS:O	1:A:223:LYS:N	2.53	0.41
2:B:339:TYR:CG	2:B:375:ILE:CD1	3.03	0.41
1:A:54:ASN:HD22	1:A:143:ARG:NH2	2.19	0.41
1:A:429:LEU:N	1:A:429:LEU:HD23	2.35	0.41
3:A:557:HBY:O1	3:A:557:HBY:H112	2.19	0.41
2:B:34:LEU:HD21	2:B:62:ALA:HB2	2.02	0.41
2:B:68:SER:O	2:B:69:THR:HG23	2.20	0.41
1:A:128:THR:OG1	1:A:146:TYR:HB2	2.20	0.41
2:B:205:LEU:O	2:B:205:LEU:HD12	2.20	0.41
2:B:34:LEU:HD12	2:B:132:ILE:HG23	2.02	0.41
1:A:188:TYR:CZ	3:A:557:HBY:H121	2.55	0.41
2:B:50:ILE:HD12	2:B:143:ARG:HG2	2.02	0.41
2:B:188:TYR:CE1	2:B:380:ILE:HG21	2.55	0.41
1:A:326:ILE:HG13	1:A:388:LYS:O	2.19	0.41
2:B:136:ASN:O	2:B:136:ASN:ND2	2.54	0.41
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.82	0.41
1:A:37:ILE:HD12	1:A:37:ILE:N	2.35	0.41
1:A:126:LYS:HE3	1:A:126:LYS:HB3	1.85	0.41
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.77	0.41
1:A:229:TRP:HD1	1:A:234:LEU:HD11	1.85	0.41
1:A:326:ILE:CG2	1:A:342:TYR:O	2.62	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TRP:C	1:A:400:THR:H	2.23	0.41
2:B:82:LYS:HD2	2:B:413:GLU:OE2	2.21	0.41
2:B:181:TYR:CD1	2:B:181:TYR:C	2.94	0.41
1:A:27:THR:HA	1:A:135:ILE:HG23	2.03	0.41
1:A:341:ILE:CD1	1:A:383:TRP:HH2	2.34	0.40
1:A:398:TRP:C	1:A:398:TRP:CD1	2.92	0.40
2:B:23:GLN:NE2	2:B:24:TRP:O	2.52	0.40
1:A:56:TYR:H	1:A:56:TYR:HD1	1.69	0.40
1:A:403:THR:HG22	1:A:403:THR:O	2.21	0.40
1:A:265:ASN:HD22	1:A:265:ASN:HA	1.53	0.40
1:A:341:ILE:HD13	1:A:383:TRP:CH2	2.57	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	Per	centil	es
1	А	554/556~(100%)	453 (82%)	75 (14%)	26~(5%)	2	14	
2	В	428/430~(100%)	342 (80%)	59 (14%)	27~(6%)		1 8	
All	All	982/986~(100%)	795 (81%)	134 (14%)	53~(5%)	2	12	

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	28	GLU
1	А	67	ASP
1	А	104	LYS
1	А	195	ILE
1	А	222	GLN
1	А	324	ASP
1	А	412	PRO



Mol	Chain	Res	Type
2	В	14	PRO
2	В	104	LYS
2	В	316	GLY
2	В	317	VAL
1	А	179	VAL
1	А	219	LYS
1	А	345	PRO
2	В	116	PHE
2	В	125	ARG
2	В	212	TRP
2	В	244	ILE
2	В	251	SER
2	В	356	ARG
2	В	427	TYR
1	А	153	TRP
1	А	184	MET
1	А	287	LYS
2	В	69	THR
2	В	98	ALA
2	В	138	GLU
2	В	153	TRP
2	В	230	MET
2	В	345	PRO
2	В	403	THR
1	А	154	LYS
1	А	236	PRO
1	А	360	ALA
2	В	66	LYS
2	В	222	GLN
1	А	244	ILE
2	В	5	ILE
2	В	195	ILE
2	В	267	ALA
1	A	271	TYR
1	А	359	GLY
1	А	4	PRO
1	А	490	GLY
2	В	236	PRO
1	A	21	VAL
2	В	156	SER
1	A	24	TRP
1	А	510	PRO



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Mol	Chain	Res	Type
2	В	148	VAL
2	В	292	VAL
1	А	156	SER
1	А	462	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
1	А	450/496~(91%)	390~(87%)	60~(13%)	4	16
2	В	363/392~(93%)	327~(90%)	36 (10%)	8	29
All	All	813/888~(92%)	717 (88%)	96 (12%)	5	21

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	4	PRO
1	А	28	GLU
1	А	29	GLU
1	А	40	GLU
1	А	42	GLU
1	А	61	PHE
1	А	65	LYS
1	А	74	LEU
1	А	76	ASP
1	А	78	ARG
1	А	79	GLU
1	А	81	ASN
1	А	97	PRO
1	А	109	LEU
1	А	113	ASP
1	А	126	LYS
1	А	135	ILE
1	А	137	ASN
1	А	164	MET



Mol	Chain	Res	Type
1	А	178	ILE
1	А	182	GLN
1	А	210	LEU
1	А	214	LEU
1	А	224	GLU
1	А	228	LEU
1	А	238	LYS
1	А	242	GLN
1	А	246	LEU
1	А	252	TRP
1	А	265	ASN
1	А	270	ILE
1	А	274	ILE
1	A	291	GLU
1	А	300	GLU
1	А	310	LEU
1	А	312	GLU
1	А	317	VAL
1	А	341	ILE
1	А	346	PHE
1	А	350	LYS
1	А	353	LYS
1	А	362	THR
1	А	364	ASP
1	А	368	LEU
1	А	431	LYS
1	А	442	VAL
1	A	448	ARG
1	А	450	THR
1	A	452	LEU
1	A	461	LYS
1	A	473	THR
1	A	474	ASN
1	A	479	LEU
1	A	484	LEU
1	A	497	THR
1	A	505	ILE
1	A	507	GLN
1	A	516	GLU
1	A	540	LYS
1	A	547	GLN
2	В	11	LYS



Mol	Chain	Res	Type
2	В	14	PRO
2	В	40	GLU
2	В	50	ILE
2	В	53	GLU
2	В	60	VAL
2	В	69	THR
2	В	74	LEU
2	В	75	VAL
2	В	86	ASP
2	В	92	LEU
2	В	163	SER
2	В	185	ASP
2	В	195	ILE
2	В	201	LYS
2	В	218	ASP
2	В	239	TRP
2	В	246	LEU
2	В	252	TRP
2	В	266	TRP
2	В	274	ILE
2	В	290	THR
2	В	311	LYS
2	В	318	TYR
2	В	324	ASP
2	В	328	GLU
2	В	330	GLN
2	В	356	ARG
2	В	362	THR
2	B	377	THR
2	В	405	TYR
2	В	409	THR
2	В	414	TRP
2	В	418	ASN
2	B	425	LEU
2	В	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	54	ASN
1	А	81	ASN
1	А	175	ASN



Mol	Chain	Res	Type
1	А	182	GLN
1	А	198	HIS
1	А	258	GLN
1	А	265	ASN
1	А	367	GLN
1	А	460	ASN
1	А	494	ASN
2	В	57	ASN
2	В	96	HIS
2	В	145	GLN
2	В	147	ASN
2	В	182	GLN
2	В	198	HIS
2	В	208	HIS
2	В	258	GLN
2	В	330	GLN
2	В	343	GLN
2	В	348	ASN
2	В	373	GLN

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).

Mal	Type	Chain	Dog	Tink	Bond lengths			Bond angles		
10101	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HBY	А	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	А	557	-	-	5/13/29/29	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	557	HBY	C1-C2	17.63	1.67	1.50
3	А	557	HBY	C9-N1	13.64	1.57	1.37
3	А	557	HBY	C3-C4	11.96	1.54	1.40
3	А	557	HBY	C2-S1	10.42	1.82	1.66
3	А	557	HBY	C1-N1	8.66	1.58	1.47
3	А	557	HBY	O3-C6	8.39	1.55	1.37
3	А	557	HBY	C7-C6	8.20	1.55	1.38
3	А	557	HBY	O1-C9	7.14	1.31	1.21
3	А	557	HBY	C2-N2	6.87	1.45	1.36
3	А	557	HBY	C8-C7	6.83	1.51	1.38
3	А	557	HBY	C13-S2	5.92	1.89	1.80
3	А	557	HBY	O2-C9	4.74	1.43	1.34
3	А	557	HBY	O2-C10	4.57	1.58	1.47
3	А	557	HBY	C3-N2	3.77	1.46	1.39
3	А	557	HBY	C8-C3	3.47	1.45	1.39
3	А	557	HBY	C13-C1	3.43	1.60	1.52
3	А	557	HBY	O3-C15	2.99	1.51	1.42
3	А	557	HBY	C4-N1	2.30	1.45	1.42
3	А	557	HBY	C5-C4	2.27	1.43	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	557	HBY	O2-C9-N1	6.23	118.10	110.81
3	А	557	HBY	C3-N2-C2	-4.84	120.51	124.74
3	А	557	HBY	O1-C9-N1	-2.86	119.29	124.09



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	А	557	HBY	O2-C10-C12	2.45	113.65	107.14
3	А	557	HBY	C14-S2-C13	-2.44	96.81	101.30
3	А	557	HBY	C2-C1-N1	2.02	115.27	110.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

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





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.

