Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 08:06 AM EDT

PDB ID	:	1BQN
Title	:	TYR 188 LEU HIV-1 RT/HBY 097
Authors	:	Hsiou, Y.; Das, K.; Ding, J.; Arnold, E.
Deposited on	:	1998-08-17
Resolution	:	3.30 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:

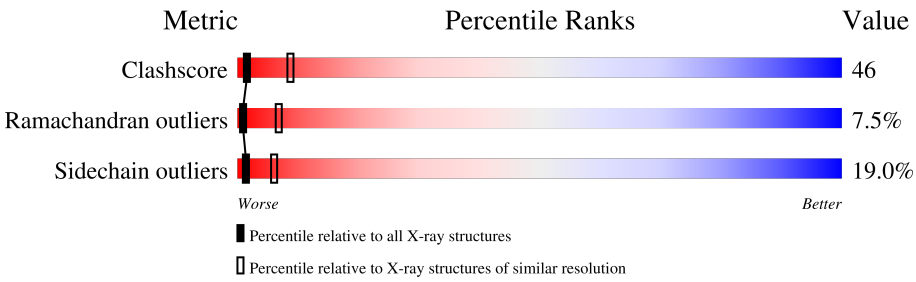
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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	558	28% 56% 14% •
2	B	430	32% 52% 14% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7834 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	558	4372	2825	729	811	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	TYR	engineered mutation	UNP P03366
A	248	GLN	GLU	conflict	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	546	GLN	GLU	conflict	UNP P03366

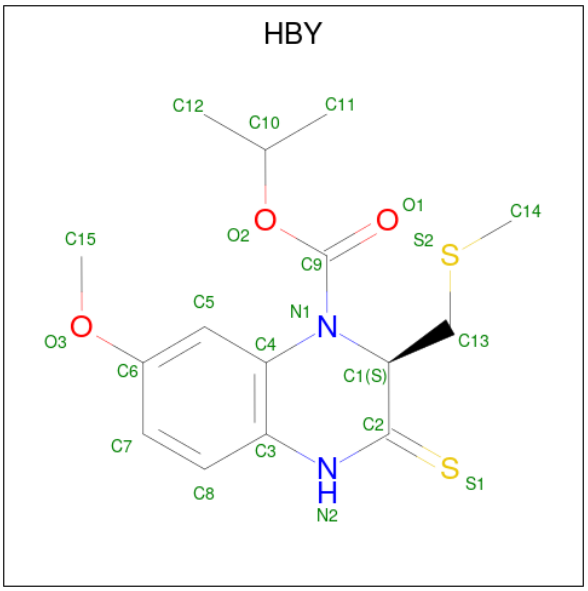
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	430	3440	2239	568	628	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	LEU	TYR	engineered mutation	UNP P03366
B	242	GLU	GLN	conflict	UNP P03366
B	278	ALA	GLN	conflict	UNP P03366
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

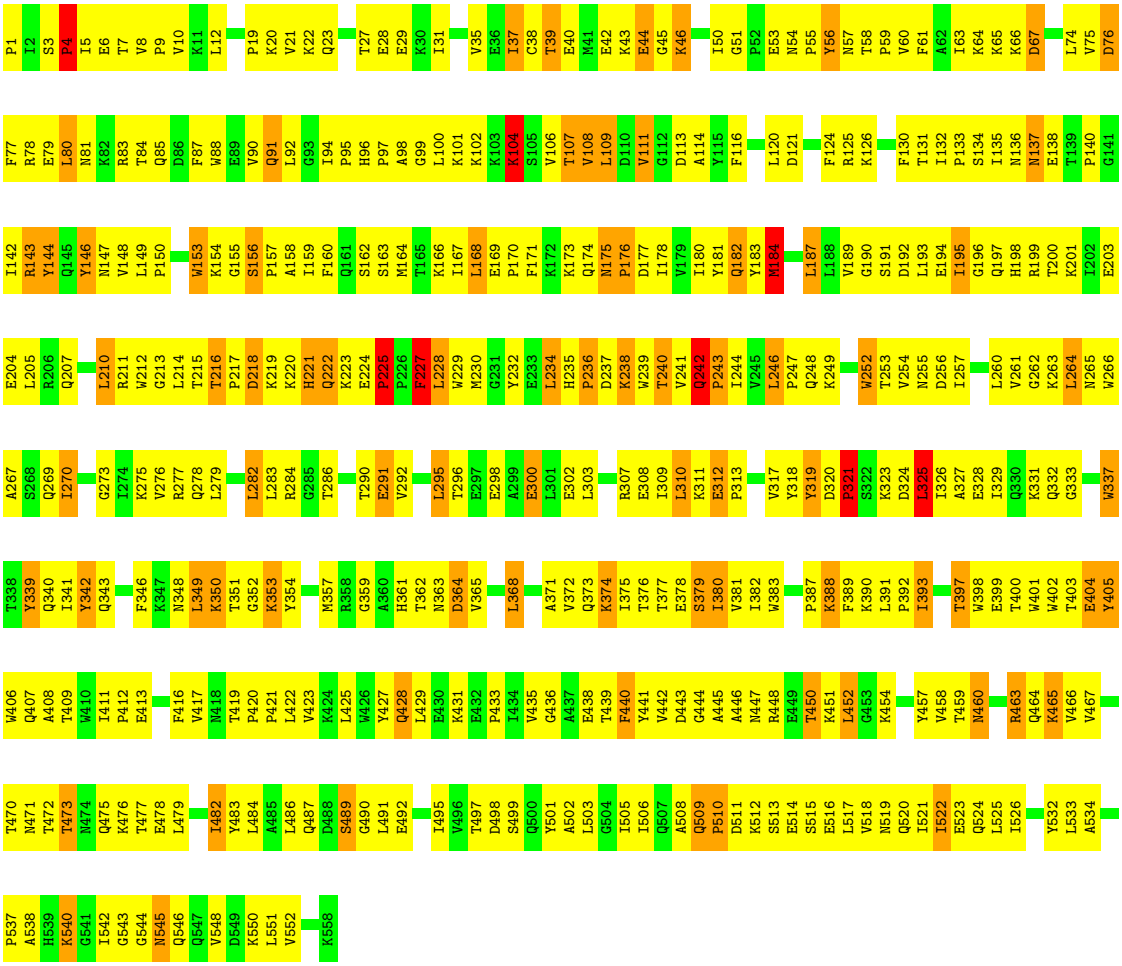
3 Residue-property plots (i)

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.

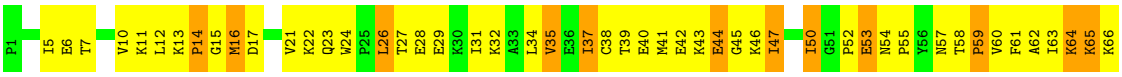
• Molecule 1: REVERSE TRANSCRIPTASE

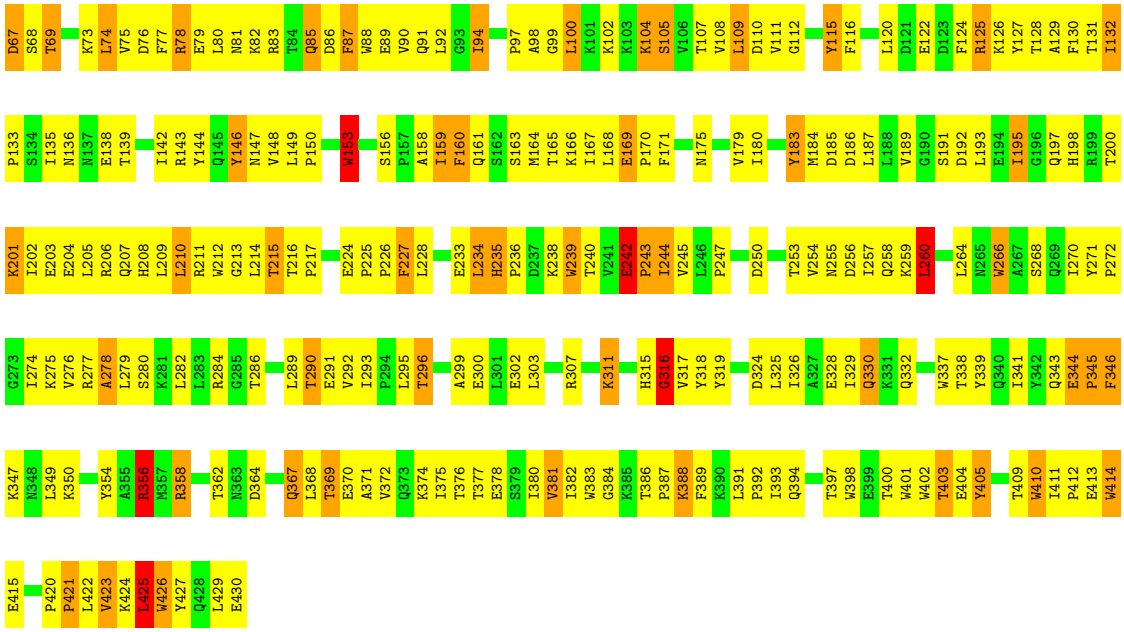
Chain A: 28% 56% 14%



• Molecule 2: REVERSE TRANSCRIPTASE

Chain B: 32% 52% 14%




D67 S68 T69 K73 L74 V75 D76 F77 R78 E79 L80 N81 K82 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 G93 I94 P97 A98 G99 L100 K101 K102 K103 K104 S105 V106 T107 V108 L109 D110 V111 G112 Y115 F116 L120 D121 E122 D123 F124 R125 K126 Y127 T128 A129 F130 T131 I132
P133 S134 I135 N136 N137 E138 T139 I142 R143 Y144 Q145 Y146 N147 V148 L149 P150 W153 S156 P157 A158 I159 F160 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 N175 V179 I180 Y183 M184 D185 D186 L187 L188 V189 G190 S191 D192 L193 E194 I195 G196 Q197 H198 R199 T200
K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 R211 W212 G213 L214 T215 T216 P217 E224 P225 P226 F227 L228 E233 L234 H235 P236 D237 K238 W239 T240 V241 E242 P243 I244 V245 L246 P247 D250 T253 V254 N255 D256 I257 Q258 K259 L260 L264 N265 W266 A267 S268 Q269 I270 Y271 P272
G273 I274 K275 V276 R277 A278 L279 S280 K281 L282 L283 R284 G285 T286 L289 T290 E291 V292 I293 P294 L295 T296 A299 E300 L301 E302 L303 R307 K311 H315 G316 V317 Y318 Y319 D324 L325 I326 A327 E328 I329 Q330 K331 Q332 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346
K347 N348 L349 K350 Y354 A355 R356 M357 R358 T362 N363 D364 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 K390 L391 P392 I393 Q394 T397 W398 E399 T400 W401 W402 T403 E404 Y405 T409 W410 I411 P412 E413 W414
E415 P420 P421 L422 V423 K424 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	224.80Å 69.30Å 105.30Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	95.1 (10.00-3.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.245 , 0.362	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7834	wwPDB-VP
Average B, all atoms (Å^2)	47.0	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	0.80	2/4487 (0.0%)	1.01	11/6118 (0.2%)
2	B	0.85	1/3539 (0.0%)	1.05	8/4825 (0.2%)
All	All	0.82	3/8026 (0.0%)	1.03	19/10943 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	514	GLU	CG-CD	6.06	1.61	1.51
1	A	337	TRP	CB-CG	-5.40	1.40	1.50
2	B	153	TRP	CB-CG	-5.09	1.41	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	316	GLY	N-CA-C	-11.27	84.93	113.10
1	A	225	PRO	N-CA-C	7.76	132.26	112.10
2	B	215	THR	N-CA-C	-7.05	91.95	111.00
2	B	94	ILE	N-CA-C	-6.68	92.97	111.00
2	B	64	LYS	N-CA-C	-6.51	93.42	111.00
1	A	184	MET	CG-SD-CE	5.95	109.72	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	344	GLU	N-CA-C	-5.67	95.69	111.00
1	A	264	LEU	CA-CB-CG	-5.61	102.39	115.30
2	B	388	LYS	N-CA-C	-5.47	96.23	111.00
2	B	426	TRP	N-CA-C	-5.43	96.33	111.00
1	A	388	LYS	N-CA-C	-5.43	96.33	111.00
1	A	80	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	227	PHE	N-CA-C	5.35	125.45	111.00
1	A	295	LEU	CA-CB-CG	-5.28	103.15	115.30
2	B	7	THR	N-CA-C	5.22	125.10	111.00
1	A	64	LYS	CB-CA-C	-5.15	100.09	110.40
1	A	109	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	310	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	325	LEU	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	TYR	Sidechain
2	B	183	TYR	Sidechain
2	B	316	GLY	Mainchain
2	B	346	PHE	Sidechain

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	4372	0	4271	410	0
2	B	3440	0	3400	313	0
3	A	22	0	20	8	0
All	All	7834	0	7691	711	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 46.

All (711) 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:41:MET:SD	2:B:41:MET:CE	2.01	1.48
1:A:97:PRO:HG2	1:A:232:TYR:CE2	1.66	1.29
1:A:27:THR:O	1:A:31:ILE:HG13	1.41	1.15
2:B:38:CYS:HB3	2:B:144:TYR:CE2	1.84	1.11
2:B:38:CYS:HB3	2:B:144:TYR:HE2	0.93	1.05
1:A:242:GLN:HB3	1:A:243:PRO:HD3	1.39	1.00
1:A:183:TYR:CE2	1:A:184:MET:HG2	1.97	1.00
1:A:229:TRP:HB3	1:A:234:LEU:HD11	1.43	0.99
1:A:191:SER:OG	1:A:198:HIS:HD2	1.47	0.98
2:B:400:THR:HG22	2:B:401:TRP:CD1	1.99	0.98
1:A:329:ILE:HD12	1:A:391:LEU:HD21	1.42	0.98
2:B:400:THR:HG22	2:B:401:TRP:HD1	1.24	0.97
1:A:108:VAL:HA	1:A:187:LEU:O	1.65	0.96
1:A:97:PRO:CG	1:A:232:TYR:CE2	2.49	0.95
1:A:40:GLU:HA	1:A:43:LYS:HB2	1.49	0.94
1:A:240:THR:HG22	1:A:241:VAL:H	1.26	0.94
2:B:125:ARG:HG2	2:B:146:TYR:O	1.71	0.91
1:A:229:TRP:HB3	1:A:234:LEU:CD1	2.00	0.90
2:B:368:LEU:O	2:B:372:VAL:HG23	1.73	0.88
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.57	0.87
2:B:242:GLU:N	2:B:243:PRO:HD3	1.90	0.86
2:B:198:HIS:O	2:B:202:ILE:HG12	1.76	0.85
1:A:10:VAL:HG12	1:A:124:PHE:HE2	1.43	0.84
1:A:278:GLN:O	1:A:282:LEU:HD23	1.76	0.84
1:A:459:THR:HG23	1:A:463:ARG:HB3	1.58	0.84
2:B:358:ARG:HH11	2:B:358:ARG:HB3	1.41	0.83
1:A:224:GLU:CB	1:A:225:PRO:HD2	2.09	0.83
1:A:107:THR:HG21	1:A:221:HIS:O	1.79	0.82
1:A:10:VAL:HG12	1:A:124:PHE:CE2	2.14	0.82
2:B:319:TYR:HD1	2:B:343:GLN:HE22	1.25	0.81
1:A:21:VAL:HG12	1:A:22:LYS:H	1.44	0.81
1:A:377:THR:O	1:A:381:VAL:HG23	1.81	0.81
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.11	0.80
2:B:23:GLN:NE2	2:B:26:LEU:HD21	1.97	0.80
1:A:183:TYR:CD2	1:A:184:MET:HG2	2.16	0.79
1:A:66:LYS:O	1:A:67:ASP:CB	2.30	0.79
1:A:3:SER:HA	1:A:213:GLY:HA3	1.64	0.79
2:B:303:LEU:O	2:B:307:ARG:HB2	1.84	0.78
1:A:438:GLU:HB3	1:A:440:PHE:HE1	1.48	0.78
2:B:423:VAL:O	2:B:425:LEU:HG	1.84	0.78
1:A:253:THR:HA	1:A:292:VAL:HA	1.65	0.78
1:A:3:SER:OG	1:A:5:ILE:HG22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD12	1:A:75:VAL:H	1.49	0.78
1:A:459:THR:CG2	1:A:463:ARG:HB3	2.13	0.78
1:A:9:PRO:HG2	2:B:53:GLU:HG2	1.64	0.78
1:A:331:LYS:HG2	1:A:333:GLY:H	1.46	0.77
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.64	0.77
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.19	0.77
1:A:97:PRO:CG	1:A:232:TYR:CD2	2.68	0.77
2:B:275:LYS:HB3	2:B:302:GLU:OE2	1.85	0.77
1:A:131:THR:HG22	1:A:143:ARG:HB3	1.67	0.76
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.65	0.76
2:B:109:LEU:HD12	2:B:187:LEU:HD23	1.69	0.75
1:A:19:PRO:O	1:A:56:TYR:HB3	1.85	0.75
2:B:341:ILE:HD12	2:B:350:LYS:HB3	1.66	0.75
2:B:167:ILE:O	2:B:208:HIS:HE1	1.70	0.75
1:A:240:THR:HG22	1:A:241:VAL:N	2.00	0.74
2:B:210:LEU:HD11	2:B:216:THR:HG23	1.69	0.74
3:A:559:HBY:C9	3:A:559:HBY:S2	2.75	0.74
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.51	0.74
1:A:27:THR:O	1:A:31:ILE:CG1	2.31	0.74
2:B:275:LYS:O	2:B:302:GLU:HB3	1.88	0.74
2:B:271:TYR:O	2:B:274:ILE:HG13	1.88	0.73
2:B:78:ARG:HD3	2:B:411:ILE:O	1.88	0.73
1:A:260:LEU:HD21	1:A:279:LEU:HD22	1.69	0.72
1:A:326:ILE:HG23	1:A:342:TYR:CE1	2.24	0.72
1:A:483:TYR:HE1	1:A:524:GLN:NE2	1.86	0.72
1:A:195:ILE:O	1:A:199:ARG:HG3	1.89	0.72
1:A:253:THR:OG1	1:A:255:ASN:HB3	1.90	0.72
1:A:325:LEU:HD11	1:A:383:TRP:CE3	2.24	0.72
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.70	0.72
1:A:132:ILE:O	1:A:142:ILE:HB	1.90	0.71
1:A:482:ILE:HG22	1:A:495:ILE:HD13	1.70	0.71
1:A:131:THR:HG22	1:A:143:ARG:HD2	1.71	0.71
1:A:401:TRP:CZ3	1:A:404:GLU:HG2	2.25	0.71
2:B:111:VAL:HG21	2:B:187:LEU:HD22	1.73	0.70
1:A:240:THR:CG2	1:A:241:VAL:H	2.04	0.70
1:A:365:VAL:O	1:A:368:LEU:HB3	1.92	0.70
2:B:375:ILE:HG13	2:B:389:PHE:CE1	2.26	0.70
1:A:382:ILE:HG23	2:B:136:ASN:OD1	1.91	0.69
1:A:454:LYS:HB2	1:A:552:VAL:HG13	1.73	0.69
1:A:518:VAL:HA	1:A:521:ILE:HD12	1.75	0.69
1:A:328:GLU:HA	1:A:390:LYS:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.20	0.69
1:A:97:PRO:HG3	1:A:232:TYR:CD2	2.28	0.68
2:B:27:THR:O	2:B:31:ILE:HG13	1.94	0.68
1:A:339:TYR:CE1	1:A:352:GLY:N	2.61	0.68
1:A:246:LEU:CD1	1:A:264:LEU:HD21	2.24	0.68
2:B:79:GLU:O	2:B:83:ARG:HG2	1.92	0.68
2:B:63:ILE:HG22	2:B:64:LYS:H	1.59	0.68
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.58	0.68
1:A:257:ILE:O	1:A:261:VAL:HG23	1.95	0.67
2:B:375:ILE:HG13	2:B:389:PHE:HE1	1.57	0.67
1:A:457:TYR:HE1	1:A:465:LYS:HD3	1.59	0.67
2:B:107:THR:OG1	2:B:198:HIS:HE1	1.77	0.67
2:B:239:TRP:N	2:B:239:TRP:HE3	1.92	0.67
2:B:243:PRO:O	2:B:245:VAL:HG23	1.95	0.67
2:B:258:GLN:NE2	2:B:289:LEU:HD21	2.10	0.67
2:B:38:CYS:CB	2:B:144:TYR:HE2	1.88	0.66
2:B:158:ALA:O	2:B:161:GLN:HB2	1.95	0.66
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.77	0.66
1:A:502:ALA:O	1:A:506:ILE:HD12	1.95	0.66
2:B:132:ILE:HG13	2:B:142:ILE:O	1.95	0.66
1:A:182:GLN:HE21	1:A:183:TYR:N	1.92	0.66
1:A:326:ILE:HG23	1:A:342:TYR:CD1	2.30	0.66
2:B:37:ILE:HG22	2:B:38:CYS:N	2.10	0.66
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.31	0.66
1:A:445:ALA:O	1:A:477:THR:HG21	1.95	0.66
2:B:369:THR:HA	2:B:398:TRP:HH2	1.61	0.66
1:A:544:GLY:HA3	2:B:286:THR:HG23	1.77	0.66
1:A:300:GLU:HA	1:A:303:LEU:HB3	1.79	0.65
1:A:483:TYR:O	1:A:486:LEU:HB2	1.95	0.65
1:A:241:VAL:HG23	1:A:270:ILE:HD11	1.77	0.65
2:B:63:ILE:HG22	2:B:64:LYS:N	2.11	0.65
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.65
1:A:4:PRO:HD2	1:A:212:TRP:O	1.97	0.65
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.79	0.65
2:B:41:MET:SD	2:B:47:ILE:HD13	2.37	0.65
1:A:57:ASN:OD1	1:A:130:PHE:HA	1.97	0.64
2:B:356:ARG:HA	2:B:356:ARG:NE	2.11	0.64
2:B:13:LYS:CB	2:B:14:PRO:HD2	2.26	0.64
2:B:128:THR:HB	2:B:146:TYR:HB2	1.78	0.64
2:B:97:PRO:O	2:B:100:LEU:HB2	1.97	0.64
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:THR:HG22	1:A:421:PRO:HD2	1.79	0.64
2:B:183:TYR:O	2:B:186:ASP:HB2	1.96	0.64
1:A:191:SER:OG	1:A:198:HIS:CD2	2.39	0.64
1:A:53:GLU:O	1:A:55:PRO:HD3	1.97	0.63
1:A:324:ASP:O	1:A:343:GLN:HG2	1.98	0.63
2:B:65:LYS:HG3	2:B:66:LYS:N	2.13	0.63
2:B:239:TRP:N	2:B:239:TRP:CE3	2.67	0.63
2:B:21:VAL:HG12	2:B:22:LYS:N	2.14	0.63
1:A:248:GLN:HG3	1:A:249:LYS:H	1.63	0.63
1:A:248:GLN:HG3	1:A:249:LYS:N	2.14	0.63
2:B:410:TRP:HE3	2:B:410:TRP:O	1.82	0.63
2:B:65:LYS:HG3	2:B:66:LYS:H	1.63	0.63
1:A:341:ILE:O	1:A:349:LEU:HB3	1.99	0.62
2:B:116:PHE:HD1	2:B:148:VAL:HG21	1.63	0.62
1:A:515:SER:OG	1:A:518:VAL:HG23	2.00	0.62
1:A:99:GLY:HA2	1:A:383:TRP:HE1	1.63	0.62
1:A:100:LEU:HD11	3:A:559:HBY:H111	1.81	0.62
1:A:77:PHE:CD1	1:A:80:LEU:HD23	2.33	0.62
1:A:246:LEU:HD12	1:A:264:LEU:HD21	1.80	0.62
1:A:483:TYR:CE1	1:A:524:GLN:NE2	2.67	0.62
1:A:216:THR:HG22	1:A:218:ASP:OD2	2.00	0.62
1:A:164:MET:CE	1:A:168:LEU:HD21	2.30	0.61
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.81	0.61
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.30	0.61
1:A:435:VAL:HG12	2:B:290:THR:HG21	1.81	0.61
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.31	0.61
1:A:428:GLN:C	1:A:429:LEU:HD23	2.21	0.61
1:A:96:HIS:CE1	1:A:98:ALA:H	2.18	0.61
2:B:425:LEU:HD12	2:B:426:TRP:H	1.64	0.61
1:A:109:LEU:HB2	1:A:187:LEU:HB3	1.83	0.61
1:A:326:ILE:HG13	1:A:388:LYS:O	1.99	0.61
2:B:164:MET:HG3	2:B:168:LEU:HD11	1.81	0.61
1:A:228:LEU:H	1:A:228:LEU:CD2	2.14	0.61
1:A:327:ALA:HB2	1:A:341:ILE:HG23	1.82	0.61
1:A:50:ILE:HG13	1:A:51:GLY:H	1.66	0.61
1:A:40:GLU:CA	1:A:43:LYS:HB2	2.28	0.60
1:A:46:LYS:HG3	1:A:148:VAL:HG21	1.83	0.60
1:A:479:LEU:O	1:A:482:ILE:HG13	2.01	0.60
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.16	0.60
1:A:12:LEU:HD23	1:A:84:THR:HA	1.83	0.60
1:A:164:MET:HE1	1:A:168:LEU:HD21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.01	0.60
1:A:5:ILE:HD12	1:A:6:GLU:HG3	1.84	0.60
2:B:78:ARG:NH1	2:B:411:ILE:HG22	2.16	0.60
2:B:164:MET:HE3	2:B:168:LEU:HG	1.84	0.60
1:A:1:PRO:HD2	1:A:44:GLU:HB3	1.82	0.60
1:A:194:GLU:O	1:A:196:GLY:N	2.35	0.60
1:A:181:TYR:OH	1:A:183:TYR:HB2	2.02	0.60
1:A:372:VAL:O	1:A:375:ILE:HB	2.01	0.60
2:B:37:ILE:CG2	2:B:38:CYS:N	2.65	0.60
1:A:429:LEU:HD13	1:A:533:LEU:HD13	1.83	0.60
2:B:50:ILE:HD11	2:B:144:TYR:C	2.22	0.60
2:B:107:THR:HG22	2:B:108:VAL:N	2.17	0.60
2:B:78:ARG:NH1	2:B:412:PRO:O	2.35	0.60
2:B:329:ILE:HG22	2:B:330:GLN:N	2.16	0.60
1:A:375:ILE:HG21	1:A:389:PHE:CZ	2.37	0.59
1:A:146:TYR:CD1	1:A:150:PRO:HG3	2.37	0.59
1:A:513:SER:HB2	1:A:519:ASN:OD1	2.02	0.59
2:B:160:PHE:O	2:B:160:PHE:CD1	2.56	0.59
1:A:244:ILE:HD11	1:A:267:ALA:HB2	1.84	0.59
1:A:265:ASN:HD21	1:A:353:LYS:NZ	2.01	0.59
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.20	0.59
1:A:460:ASN:H	1:A:460:ASN:HD22	1.49	0.59
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.68	0.59
2:B:126:LYS:HG3	2:B:127:TYR:CE1	2.37	0.59
2:B:242:GLU:H	2:B:243:PRO:HD3	1.68	0.59
2:B:344:GLU:O	2:B:347:LYS:HB2	2.03	0.58
1:A:114:ALA:O	1:A:160:PHE:HE2	1.86	0.58
1:A:153:TRP:HZ3	1:A:159:ILE:HD12	1.68	0.58
1:A:166:LYS:O	1:A:169:GLU:HB3	2.03	0.58
2:B:303:LEU:HD21	2:B:307:ARG:NH1	2.18	0.58
1:A:484:LEU:HA	1:A:487:GLN:OE1	2.04	0.58
2:B:391:LEU:HD12	2:B:414:TRP:HB2	1.85	0.58
2:B:375:ILE:HG21	2:B:389:PHE:CZ	2.38	0.58
2:B:329:ILE:HG23	2:B:338:THR:O	2.04	0.58
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.34	0.58
1:A:254:VAL:CG1	1:A:283:LEU:HD11	2.34	0.58
2:B:132:ILE:HG22	2:B:133:PRO:HD2	1.85	0.58
2:B:257:ILE:HD13	2:B:282:LEU:HD23	1.85	0.58
2:B:319:TYR:CD2	2:B:383:TRP:CD1	2.92	0.58
1:A:96:HIS:CD2	1:A:232:TYR:OH	2.57	0.57
1:A:483:TYR:HE1	1:A:524:GLN:HE21	1.49	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LYS:C	2:B:239:TRP:HE3	2.08	0.57
2:B:244:ILE:HG22	2:B:244:ILE:O	2.04	0.57
2:B:260:LEU:O	2:B:264:LEU:HG	2.03	0.57
2:B:268:SER:O	2:B:272:PRO:HA	2.05	0.57
1:A:56:TYR:CD1	1:A:56:TYR:N	2.69	0.57
1:A:106:VAL:HG13	1:A:189:VAL:O	2.05	0.57
1:A:46:LYS:HG2	1:A:116:PHE:HD2	1.68	0.57
1:A:253:THR:O	1:A:257:ILE:HG13	2.04	0.57
2:B:115:TYR:N	2:B:115:TYR:CD1	2.72	0.57
1:A:171:PHE:CD1	1:A:175:ASN:OD1	2.58	0.56
2:B:410:TRP:O	2:B:410:TRP:CE3	2.58	0.56
1:A:235:HIS:ND1	1:A:238:LYS:HG3	2.20	0.56
1:A:266:TRP:CH2	1:A:269:GLN:NE2	2.73	0.56
1:A:131:THR:HG22	1:A:143:ARG:CD	2.35	0.56
2:B:61:PHE:HD2	2:B:74:LEU:HD23	1.69	0.56
1:A:483:TYR:HE1	1:A:524:GLN:CG	2.18	0.56
2:B:10:VAL:HA	2:B:88:TRP:CZ2	2.39	0.56
2:B:254:VAL:HB	2:B:289:LEU:HD23	1.87	0.56
1:A:116:PHE:O	1:A:148:VAL:HG21	2.06	0.56
1:A:254:VAL:HA	1:A:257:ILE:HD12	1.86	0.56
2:B:79:GLU:HG3	2:B:83:ARG:NH1	2.20	0.56
1:A:100:LEU:HD11	3:A:559:HBY:C11	2.35	0.56
2:B:329:ILE:HA	2:B:338:THR:O	2.06	0.56
1:A:363:ASN:OD1	1:A:364:ASP:N	2.39	0.56
2:B:264:LEU:HD13	2:B:276:VAL:CG1	2.36	0.56
1:A:114:ALA:O	1:A:160:PHE:CE2	2.59	0.56
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.35	0.55
1:A:21:VAL:HG12	1:A:22:LYS:N	2.17	0.55
1:A:375:ILE:CG2	1:A:389:PHE:HZ	2.20	0.55
1:A:501:TYR:O	1:A:505:ILE:HG13	2.06	0.55
2:B:247:PRO:HB2	2:B:250:ASP:CB	2.36	0.55
2:B:17:ASP:O	2:B:83:ARG:NE	2.39	0.55
2:B:125:ARG:HE	2:B:147:ASN:HA	1.71	0.55
2:B:131:THR:HG22	2:B:132:ILE:N	2.21	0.55
1:A:341:ILE:HD12	1:A:350:LYS:HB3	1.88	0.55
1:A:108:VAL:CA	1:A:187:LEU:O	2.46	0.55
2:B:225:PRO:N	2:B:226:PRO:HD2	2.20	0.55
2:B:377:THR:O	2:B:381:VAL:HG23	2.06	0.55
1:A:319:TYR:CD1	1:A:320:ASP:N	2.74	0.55
1:A:422:LEU:HG	1:A:423:VAL:N	2.21	0.55
1:A:319:TYR:HE1	1:A:343:GLN:NE2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HA	1:A:375:ILE:HD12	1.89	0.55
1:A:144:TYR:N	1:A:144:TYR:CD1	2.75	0.55
1:A:427:TYR:OH	1:A:509:GLN:HA	2.07	0.55
3:A:559:HBY:S2	3:A:559:HBY:O1	2.65	0.55
2:B:191:SER:OG	2:B:198:HIS:HD2	1.89	0.55
1:A:337:TRP:N	1:A:337:TRP:CD1	2.76	0.54
1:A:398:TRP:O	1:A:400:THR:N	2.39	0.54
1:A:508:ALA:O	1:A:509:GLN:HG2	2.07	0.54
2:B:12:LEU:HD13	2:B:16:MET:O	2.07	0.54
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.42	0.54
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.07	0.54
1:A:420:PRO:HG2	1:A:421:PRO:HD2	1.89	0.54
2:B:136:ASN:O	2:B:136:ASN:ND2	2.41	0.54
1:A:509:GLN:N	1:A:510:PRO:HD3	2.22	0.54
2:B:26:LEU:HG	2:B:133:PRO:HG3	1.90	0.54
2:B:23:GLN:HE22	2:B:26:LEU:HD21	1.72	0.54
1:A:464:GLN:O	1:A:465:LYS:HB2	2.07	0.54
1:A:228:LEU:H	1:A:228:LEU:HD23	1.72	0.54
2:B:81:ASN:N	2:B:81:ASN:OD1	2.38	0.54
2:B:109:LEU:HB2	2:B:111:VAL:HG23	1.89	0.54
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.90	0.54
1:A:373:GLN:O	1:A:375:ILE:N	2.41	0.54
2:B:59:PRO:HB2	2:B:76:ASP:CB	2.37	0.54
2:B:367:GLN:O	2:B:371:ALA:N	2.40	0.54
2:B:394:GLN:HB3	2:B:397:THR:HB	1.88	0.54
1:A:1:PRO:CD	1:A:44:GLU:HG2	2.37	0.54
1:A:521:ILE:HG22	1:A:525:LEU:HD12	1.89	0.54
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.43	0.53
1:A:170:PRO:O	1:A:173:LYS:HB3	2.08	0.53
1:A:200:THR:OG1	1:A:201:LYS:N	2.41	0.53
1:A:319:TYR:CD2	1:A:383:TRP:HD1	2.26	0.53
1:A:375:ILE:HD13	1:A:389:PHE:HE1	1.74	0.53
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.43	0.53
1:A:131:THR:C	1:A:133:PRO:HD3	2.28	0.53
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.44	0.53
2:B:40:GLU:O	2:B:43:LYS:HB2	2.08	0.53
1:A:109:LEU:N	1:A:187:LEU:O	2.41	0.53
1:A:275:LYS:HE2	1:A:332:GLN:HE21	1.73	0.53
1:A:521:ILE:HG22	1:A:525:LEU:CD1	2.39	0.53
1:A:482:ILE:CG2	1:A:495:ILE:HD13	2.39	0.53
2:B:124:PHE:O	2:B:126:LYS:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:PRO:HD2	1:A:44:GLU:HG2	1.90	0.53
1:A:96:HIS:N	2:B:136:ASN:HD21	2.06	0.53
2:B:193:LEU:HD13	2:B:197:GLN:HB3	1.89	0.53
2:B:356:ARG:HA	2:B:356:ARG:HE	1.73	0.53
1:A:354:TYR:CD2	1:A:371:ALA:HB2	2.44	0.53
2:B:85:GLN:O	2:B:89:GLU:HB2	2.09	0.53
1:A:429:LEU:HD23	1:A:429:LEU:N	2.24	0.53
1:A:153:TRP:HE3	1:A:156:SER:H	1.56	0.52
1:A:178:ILE:HD11	1:A:189:VAL:HG12	1.89	0.52
1:A:342:TYR:HD1	1:A:342:TYR:O	1.92	0.52
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.39	0.52
2:B:126:LYS:HG3	2:B:127:TYR:CD1	2.44	0.52
2:B:234:LEU:O	2:B:236:PRO:HD3	2.09	0.52
2:B:282:LEU:HD13	2:B:296:THR:HG22	1.92	0.52
1:A:111:VAL:O	1:A:114:ALA:HB3	2.08	0.52
2:B:78:ARG:CZ	2:B:411:ILE:HG22	2.39	0.52
1:A:101:LYS:NZ	1:A:321:PRO:HG3	2.25	0.52
1:A:193:LEU:O	1:A:198:HIS:HB2	2.09	0.52
1:A:279:LEU:HD12	1:A:302:GLU:OE1	2.10	0.52
1:A:100:LEU:CD1	3:A:559:HBY:H111	2.40	0.52
1:A:109:LEU:HD23	1:A:218:ASP:OD2	2.09	0.52
1:A:131:THR:O	1:A:133:PRO:HD3	2.10	0.52
1:A:393:ILE:HD13	1:A:398:TRP:HE3	1.75	0.52
1:A:96:HIS:HD2	1:A:232:TYR:OH	1.93	0.52
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.39	0.52
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.92	0.52
2:B:278:ALA:O	2:B:299:ALA:HB2	2.10	0.52
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.92	0.52
1:A:420:PRO:HG2	1:A:421:PRO:CD	2.39	0.52
2:B:179:VAL:HG12	2:B:180:ILE:N	2.25	0.52
1:A:393:ILE:CD1	1:A:398:TRP:HE3	2.23	0.51
2:B:6:GLU:OE1	2:B:6:GLU:HA	2.10	0.51
1:A:196:GLY:O	1:A:200:THR:HG23	2.11	0.51
1:A:339:TYR:HD1	1:A:339:TYR:O	1.91	0.51
1:A:466:VAL:HG12	1:A:467:VAL:N	2.24	0.51
2:B:107:THR:HG22	2:B:108:VAL:H	1.75	0.51
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.93	0.51
2:B:277:ARG:O	2:B:279:LEU:N	2.43	0.51
1:A:12:LEU:HA	1:A:84:THR:HA	1.92	0.51
1:A:244:ILE:O	1:A:244:ILE:HG23	2.11	0.51
2:B:424:LYS:O	2:B:425:LEU:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.92	0.51
1:A:5:ILE:HD12	1:A:6:GLU:H	1.76	0.51
1:A:252:TRP:N	1:A:252:TRP:CD1	2.78	0.51
2:B:191:SER:OG	2:B:198:HIS:CD2	2.63	0.51
1:A:511:ASP:O	1:A:522:ILE:HD13	2.10	0.51
2:B:79:GLU:CG	2:B:83:ARG:NH1	2.74	0.51
1:A:354:TYR:HD2	1:A:371:ALA:HB2	1.75	0.51
1:A:447:ASN:CB	1:A:450:THR:OG1	2.59	0.51
2:B:68:SER:O	2:B:69:THR:HG23	2.11	0.51
1:A:381:VAL:O	1:A:381:VAL:HG12	2.11	0.51
1:A:342:TYR:CD1	1:A:342:TYR:O	2.64	0.50
1:A:490:GLY:O	1:A:491:LEU:HD23	2.11	0.50
1:A:42:GLU:O	1:A:45:GLY:HA2	2.11	0.50
1:A:224:GLU:CB	1:A:225:PRO:CD	2.87	0.50
1:A:419:THR:HG23	1:A:420:PRO:HD2	1.93	0.50
2:B:128:THR:CB	2:B:146:TYR:HB2	2.41	0.50
1:A:116:PHE:O	1:A:148:VAL:HG11	2.11	0.50
1:A:375:ILE:HG21	1:A:389:PHE:HZ	1.74	0.50
1:A:121:ASP:O	1:A:125:ARG:HG3	2.11	0.50
1:A:397:THR:HG21	1:A:425:LEU:H	1.77	0.50
2:B:164:MET:HE2	2:B:168:LEU:HD21	1.92	0.50
1:A:59:PRO:O	1:A:75:VAL:HG13	2.11	0.50
1:A:340:GLN:HA	1:A:351:THR:HG22	1.92	0.50
1:A:544:GLY:HA2	2:B:284:ARG:O	2.11	0.50
2:B:193:LEU:HD11	2:B:201:LYS:HG2	1.93	0.50
2:B:258:GLN:HE22	2:B:289:LEU:HD21	1.72	0.50
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.10	0.50
2:B:364:ASP:O	2:B:367:GLN:HB2	2.12	0.50
1:A:153:TRP:O	1:A:155:GLY:N	2.45	0.50
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.77	0.50
2:B:282:LEU:HD22	2:B:295:LEU:HA	1.93	0.50
1:A:339:TYR:CD1	1:A:339:TYR:C	2.86	0.50
1:A:373:GLN:O	1:A:376:THR:N	2.44	0.50
2:B:200:THR:O	2:B:202:ILE:N	2.44	0.50
2:B:224:GLU:HB3	2:B:226:PRO:HD2	1.94	0.50
2:B:326:ILE:HG12	2:B:388:LYS:HB3	1.93	0.50
2:B:376:THR:O	2:B:380:ILE:HG12	2.11	0.50
1:A:326:ILE:HG22	1:A:342:TYR:O	2.12	0.49
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.47	0.49
2:B:398:TRP:C	2:B:400:THR:H	2.14	0.49
1:A:9:PRO:CG	2:B:53:GLU:HG2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:O	1:A:374:LYS:C	2.50	0.49
1:A:365:VAL:HG11	1:A:401:TRP:HB3	1.94	0.49
1:A:458:VAL:HA	1:A:463:ARG:O	2.11	0.49
1:A:391:LEU:CD2	1:A:392:PRO:HD2	2.43	0.49
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.47	0.49
1:A:241:VAL:HG11	1:A:266:TRP:HE1	1.77	0.49
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.11	0.49
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.48	0.49
1:A:46:LYS:CG	1:A:148:VAL:HG21	2.42	0.49
1:A:56:TYR:H	1:A:56:TYR:HD1	1.58	0.49
1:A:219:LYS:O	1:A:221:HIS:N	2.45	0.49
2:B:102:LYS:HA	2:B:102:LYS:HE2	1.94	0.49
1:A:339:TYR:HD1	1:A:339:TYR:C	2.16	0.49
1:A:476:LYS:O	1:A:479:LEU:HB3	2.12	0.49
1:A:225:PRO:HG3	1:A:236:PRO:HG3	1.94	0.49
1:A:373:GLN:OE1	2:B:400:THR:HG21	2.12	0.49
2:B:34:LEU:HD21	2:B:62:ALA:HB2	1.95	0.49
1:A:37:ILE:HG22	1:A:38:CYS:N	2.28	0.49
2:B:277:ARG:O	2:B:280:SER:N	2.45	0.49
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.94	0.48
1:A:132:ILE:O	1:A:142:ILE:HD12	2.12	0.48
1:A:379:SER:CB	1:A:387:PRO:HD3	2.43	0.48
1:A:517:LEU:O	1:A:521:ILE:HG13	2.13	0.48
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.95	0.48
1:A:19:PRO:HD3	1:A:83:ARG:HD3	1.94	0.48
1:A:96:HIS:CE1	1:A:98:ALA:HB3	2.47	0.48
1:A:326:ILE:HG12	1:A:327:ALA:N	2.27	0.48
1:A:457:TYR:O	1:A:458:VAL:HG23	2.13	0.48
1:A:483:TYR:HE2	1:A:520:GLN:NE2	2.12	0.48
2:B:202:ILE:O	2:B:205:LEU:N	2.45	0.48
2:B:234:LEU:HD12	2:B:381:VAL:HG21	1.95	0.48
1:A:43:LYS:C	1:A:45:GLY:H	2.16	0.48
2:B:41:MET:HG3	2:B:46:LYS:HD2	1.95	0.48
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.47	0.48
1:A:120:LEU:HD13	1:A:149:LEU:HD23	1.95	0.48
1:A:398:TRP:C	1:A:400:THR:N	2.65	0.48
2:B:210:LEU:HD12	2:B:215:THR:O	2.13	0.48
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.48	0.48
1:A:95:PRO:HB2	2:B:136:ASN:ND2	2.28	0.48
1:A:144:TYR:N	1:A:144:TYR:HD1	2.11	0.48
2:B:125:ARG:NE	2:B:147:ASN:HA	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:HG22	1:A:40:GLU:N	2.28	0.48
1:A:265:ASN:ND2	1:A:353:LYS:NZ	2.60	0.48
2:B:32:LYS:O	2:B:35:VAL:HG23	2.14	0.48
2:B:126:LYS:HE3	2:B:127:TYR:CE1	2.48	0.48
2:B:193:LEU:HB3	2:B:197:GLN:HB2	1.96	0.48
1:A:379:SER:OG	1:A:387:PRO:CG	2.62	0.48
2:B:264:LEU:HD13	2:B:276:VAL:HG12	1.94	0.48
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.49	0.48
2:B:59:PRO:O	2:B:75:VAL:HG12	2.14	0.48
2:B:31:ILE:HG12	2:B:133:PRO:HG2	1.96	0.48
2:B:59:PRO:HB2	2:B:76:ASP:HB2	1.94	0.48
2:B:131:THR:CG2	2:B:132:ILE:N	2.77	0.48
2:B:319:TYR:CE2	2:B:383:TRP:HD1	2.31	0.48
1:A:252:TRP:HD1	1:A:252:TRP:H	1.62	0.48
1:A:298:GLU:OE1	1:A:298:GLU:HA	2.14	0.48
1:A:31:ILE:HD13	1:A:134:SER:HA	1.95	0.47
1:A:178:ILE:HD11	1:A:189:VAL:CG1	2.44	0.47
2:B:242:GLU:N	2:B:243:PRO:CD	2.70	0.47
2:B:256:ASP:O	2:B:259:LYS:HB2	2.14	0.47
2:B:107:THR:OG1	2:B:198:HIS:CE1	2.64	0.47
2:B:159:ILE:O	2:B:161:GLN:N	2.48	0.47
1:A:483:TYR:CE1	1:A:524:GLN:CG	2.97	0.47
2:B:328:GLU:O	2:B:339:TYR:HA	2.14	0.47
2:B:368:LEU:HD23	2:B:398:TRP:CZ3	2.48	0.47
1:A:21:VAL:CG1	1:A:22:LYS:H	2.22	0.47
1:A:522:ILE:HG22	1:A:523:GLU:N	2.30	0.47
2:B:354:TYR:CE1	2:B:374:LYS:HD2	2.49	0.47
1:A:181:TYR:CD1	1:A:181:TYR:C	2.88	0.47
1:A:248:GLN:CG	1:A:249:LYS:N	2.77	0.47
1:A:532:TYR:CE1	1:A:533:LEU:O	2.67	0.47
1:A:101:LYS:HE2	1:A:321:PRO:HD3	1.95	0.47
2:B:325:LEU:HD21	2:B:349:LEU:HD13	1.96	0.47
1:A:246:LEU:HB3	1:A:263:LYS:HD2	1.96	0.47
1:A:473:THR:OG1	1:A:476:LYS:HB2	2.15	0.47
2:B:266:TRP:CE3	2:B:266:TRP:CA	2.96	0.47
1:A:227:PHE:O	1:A:234:LEU:HD12	2.15	0.47
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.98	0.47
1:A:391:LEU:HD23	1:A:392:PRO:HD2	1.97	0.47
1:A:552:VAL:HG12	1:A:552:VAL:O	2.15	0.47
2:B:224:GLU:HB2	2:B:228:LEU:HD12	1.96	0.47
2:B:329:ILE:HG22	2:B:330:GLN:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:ILE:O	2:B:378:GLU:HB2	2.15	0.47
1:A:522:ILE:O	1:A:525:LEU:HB2	2.15	0.47
2:B:43:LYS:O	2:B:45:GLY:N	2.47	0.47
2:B:369:THR:HA	2:B:398:TRP:CH2	2.47	0.47
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.97	0.46
2:B:148:VAL:HG23	2:B:149:LEU:N	2.30	0.46
2:B:167:ILE:O	2:B:208:HIS:CE1	2.59	0.46
1:A:87:PHE:CE2	1:A:155:GLY:CA	2.98	0.46
1:A:153:TRP:HE3	1:A:156:SER:N	2.14	0.46
1:A:542:ILE:HG12	1:A:545:ASN:CG	2.35	0.46
2:B:21:VAL:CG1	2:B:22:LYS:N	2.79	0.46
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.97	0.46
2:B:161:GLN:O	2:B:164:MET:N	2.48	0.46
2:B:282:LEU:HD13	2:B:296:THR:CG2	2.45	0.46
1:A:106:VAL:CG1	1:A:107:THR:N	2.78	0.46
1:A:155:GLY:O	1:A:156:SER:C	2.54	0.46
2:B:13:LYS:O	2:B:15:GLY:N	2.49	0.46
1:A:74:LEU:CD1	1:A:75:VAL:H	2.25	0.46
1:A:486:LEU:HD11	1:A:521:ILE:HG23	1.97	0.46
2:B:184:MET:HG2	2:B:410:TRP:HD1	1.80	0.46
2:B:325:LEU:O	2:B:387:PRO:HA	2.16	0.46
2:B:424:LYS:O	2:B:426:TRP:N	2.48	0.46
1:A:543:GLY:C	1:A:545:ASN:H	2.19	0.46
1:A:8:VAL:O	1:A:121:ASP:HB2	2.16	0.46
1:A:90:VAL:O	1:A:92:LEU:N	2.48	0.46
1:A:323:LYS:O	1:A:343:GLN:NE2	2.49	0.46
1:A:342:TYR:CD1	1:A:342:TYR:C	2.89	0.46
1:A:400:THR:O	1:A:404:GLU:N	2.48	0.46
2:B:5:ILE:HG22	2:B:6:GLU:N	2.31	0.46
2:B:260:LEU:O	2:B:260:LEU:HD12	2.16	0.46
2:B:369:THR:HG23	2:B:398:TRP:CH2	2.51	0.46
2:B:392:PRO:O	2:B:393:ILE:HB	2.15	0.46
1:A:201:LYS:HA	1:A:204:GLU:HB2	1.98	0.46
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.97	0.46
2:B:27:THR:HG22	2:B:29:GLU:H	1.81	0.46
2:B:124:PHE:CE2	2:B:153:TRP:CH2	3.03	0.46
2:B:115:TYR:N	2:B:115:TYR:HD1	2.14	0.46
2:B:159:ILE:C	2:B:161:GLN:H	2.20	0.46
2:B:216:THR:HA	2:B:217:PRO:HD3	1.86	0.46
2:B:120:LEU:HD11	2:B:124:PHE:CD2	2.51	0.46
1:A:326:ILE:HD11	1:A:390:LYS:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:HA	1:A:510:PRO:HA	1.98	0.45
2:B:183:TYR:CE2	2:B:380:ILE:HD12	2.51	0.45
2:B:346:PHE:HA	2:B:430:GLU:OXT	2.17	0.45
1:A:307:ARG:O	1:A:311:LYS:N	2.49	0.45
2:B:31:ILE:CG2	2:B:133:PRO:O	2.65	0.45
2:B:105:SER:O	2:B:198:HIS:NE2	2.49	0.45
1:A:79:GLU:HG2	1:A:83:ARG:NH1	2.31	0.45
1:A:79:GLU:O	1:A:83:ARG:HD2	2.15	0.45
1:A:87:PHE:C	2:B:55:PRO:HB3	2.37	0.45
2:B:116:PHE:HD1	2:B:148:VAL:CG2	2.30	0.45
1:A:153:TRP:HB3	1:A:156:SER:OG	2.16	0.45
2:B:54:ASN:C	2:B:54:ASN:OD1	2.55	0.45
2:B:100:LEU:HG	2:B:381:VAL:O	2.16	0.45
2:B:238:LYS:HB2	2:B:239:TRP:CZ3	2.51	0.45
2:B:405:TYR:CD1	2:B:405:TYR:N	2.83	0.45
1:A:180:ILE:CG2	1:A:187:LEU:HD11	2.47	0.45
1:A:339:TYR:O	1:A:339:TYR:CD1	2.69	0.45
3:A:559:HBY:O2	3:A:559:HBY:H5	2.17	0.45
1:A:235:HIS:O	1:A:237:ASP:N	2.49	0.45
1:A:343:GLN:HG3	1:A:349:LEU:CD2	2.47	0.45
1:A:508:ALA:C	1:A:509:GLN:HG2	2.37	0.45
1:A:513:SER:O	1:A:519:ASN:ND2	2.49	0.45
2:B:23:GLN:HE21	2:B:26:LEU:HD21	1.76	0.45
2:B:115:TYR:OH	2:B:185:ASP:HA	2.17	0.45
2:B:402:TRP:C	2:B:404:GLU:N	2.70	0.45
1:A:465:LYS:O	1:A:466:VAL:HG23	2.17	0.45
1:A:466:VAL:CG1	1:A:467:VAL:N	2.79	0.45
2:B:73:LYS:NZ	2:B:130:PHE:CE2	2.79	0.45
2:B:99:GLY:O	2:B:102:LYS:HB2	2.17	0.45
2:B:184:MET:HG2	2:B:410:TRP:CD1	2.51	0.45
2:B:264:LEU:HB3	2:B:276:VAL:HG11	1.99	0.45
2:B:425:LEU:CD1	2:B:426:TRP:H	2.30	0.45
1:A:483:TYR:HE1	1:A:524:GLN:CD	2.18	0.45
2:B:37:ILE:HG22	2:B:38:CYS:H	1.80	0.45
1:A:43:LYS:C	1:A:45:GLY:N	2.71	0.45
1:A:76:ASP:O	1:A:78:ARG:HG2	2.17	0.45
1:A:190:GLY:HA3	3:A:559:HBY:C14	2.47	0.45
2:B:200:THR:C	2:B:202:ILE:N	2.68	0.45
1:A:176:PRO:HG2	1:A:177:ASP:H	1.81	0.44
1:A:218:ASP:HB3	1:A:222:GLN:CB	2.47	0.44
1:A:379:SER:HB3	1:A:387:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLY:O	1:A:445:ALA:HB2	2.17	0.44
2:B:210:LEU:HD12	2:B:210:LEU:HA	1.60	0.44
2:B:330:GLN:CG	2:B:338:THR:OG1	2.63	0.44
1:A:326:ILE:CG2	1:A:342:TYR:O	2.65	0.44
1:A:153:TRP:CE3	1:A:156:SER:N	2.85	0.44
1:A:492:GLU:O	1:A:492:GLU:HG3	2.17	0.44
2:B:34:LEU:HD21	2:B:61:PHE:O	2.18	0.44
2:B:80:LEU:HD23	2:B:153:TRP:CD1	2.52	0.44
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.72	0.44
1:A:96:HIS:ND1	1:A:98:ALA:HB3	2.33	0.44
1:A:160:PHE:CD1	1:A:160:PHE:C	2.91	0.44
2:B:21:VAL:HG12	2:B:22:LYS:H	1.82	0.44
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.60	0.44
1:A:210:LEU:HD22	1:A:215:THR:HA	2.00	0.44
1:A:440:PHE:N	1:A:440:PHE:CD1	2.86	0.44
2:B:160:PHE:O	2:B:161:GLN:C	2.55	0.44
1:A:447:ASN:N	1:A:452:LEU:O	2.50	0.44
2:B:60:VAL:CG1	2:B:73:LYS:HE3	2.48	0.44
1:A:229:TRP:CB	1:A:234:LEU:CD1	2.86	0.44
2:B:210:LEU:O	2:B:214:LEU:N	2.50	0.44
1:A:181:TYR:CD1	1:A:182:GLN:N	2.86	0.43
1:A:312:GLU:HA	1:A:313:PRO:HD2	1.45	0.43
1:A:522:ILE:CG2	1:A:523:GLU:N	2.81	0.43
2:B:87:PHE:CZ	2:B:91:GLN:NE2	2.86	0.43
2:B:179:VAL:O	2:B:180:ILE:HG13	2.18	0.43
2:B:235:HIS:O	2:B:239:TRP:CZ3	2.71	0.43
2:B:329:ILE:CG2	2:B:330:GLN:N	2.80	0.43
1:A:170:PRO:O	1:A:174:GLN:N	2.49	0.43
1:A:99:GLY:CA	1:A:383:TRP:HE1	2.31	0.43
1:A:265:ASN:HD21	1:A:353:LYS:HZ1	1.64	0.43
1:A:373:GLN:C	1:A:375:ILE:N	2.68	0.43
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.53	0.43
1:A:470:THR:O	1:A:472:THR:HG23	2.18	0.43
1:A:486:LEU:O	1:A:489:SER:OG	2.28	0.43
2:B:343:GLN:HE21	2:B:349:LEU:CD1	2.30	0.43
1:A:8:VAL:HG11	2:B:52:PRO:HG2	1.99	0.43
1:A:181:TYR:HH	1:A:229:TRP:HH2	1.65	0.43
1:A:546:GLN:O	1:A:550:LYS:CB	2.66	0.43
2:B:63:ILE:CG2	2:B:64:LYS:N	2.80	0.43
2:B:109:LEU:HD22	2:B:206:ARG:HE	1.84	0.43
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ILE:HG22	1:A:495:ILE:CD1	2.41	0.43
1:A:273:GLY:O	1:A:309:ILE:HD13	2.19	0.43
1:A:498:ASP:OD1	1:A:542:ILE:HG21	2.19	0.43
2:B:57:ASN:OD1	2:B:58:THR:N	2.47	0.43
2:B:120:LEU:HD23	2:B:125:ARG:CG	2.48	0.43
2:B:330:GLN:HE21	2:B:330:GLN:HB3	1.63	0.43
1:A:442:VAL:CG2	1:A:495:ILE:HG23	2.48	0.43
2:B:39:THR:O	2:B:42:GLU:HB3	2.19	0.43
1:A:136:ASN:O	1:A:138:GLU:N	2.52	0.43
2:B:94:ILE:HD11	2:B:158:ALA:HA	2.01	0.43
2:B:156:SER:O	2:B:158:ALA:N	2.50	0.43
2:B:227:PHE:CG	2:B:227:PHE:O	2.72	0.43
2:B:343:GLN:NE2	2:B:349:LEU:HD11	2.33	0.43
2:B:90:VAL:HB	2:B:91:GLN:H	1.54	0.43
2:B:422:LEU:O	2:B:425:LEU:HD23	2.18	0.43
1:A:446:ALA:HA	1:A:452:LEU:O	2.19	0.43
1:A:470:THR:HG22	1:A:471:ASN:N	2.34	0.43
1:A:473:THR:C	1:A:475:GLN:N	2.71	0.43
2:B:354:TYR:CD1	2:B:374:LYS:HD2	2.53	0.43
1:A:229:TRP:NE1	3:A:559:HBY:H113	2.34	0.42
1:A:262:GLY:O	1:A:265:ASN:HB2	2.19	0.42
1:A:400:THR:C	1:A:402:TRP:H	2.23	0.42
2:B:402:TRP:C	2:B:404:GLU:H	2.22	0.42
2:B:264:LEU:HD13	2:B:276:VAL:HG11	2.01	0.42
2:B:337:TRP:O	2:B:338:THR:HG23	2.19	0.42
2:B:343:GLN:HE21	2:B:349:LEU:HD11	1.83	0.42
2:B:26:LEU:CD1	2:B:133:PRO:HG3	2.49	0.42
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.49	0.42
1:A:317:VAL:HG22	1:A:318:TYR:H	1.84	0.42
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.54	0.42
2:B:205:LEU:O	2:B:205:LEU:HD12	2.18	0.42
1:A:74:LEU:HD12	1:A:75:VAL:N	2.27	0.42
1:A:265:ASN:HD21	1:A:353:LYS:HZ2	1.68	0.42
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.87	0.42
2:B:193:LEU:HB2	2:B:198:HIS:HB2	2.01	0.42
2:B:391:LEU:HB2	2:B:415:GLU:O	2.19	0.42
1:A:10:VAL:HG13	1:A:85:GLN:HG2	2.02	0.42
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.77	0.42
2:B:82:LYS:HD2	2:B:413:GLU:OE2	2.20	0.42
1:A:106:VAL:HG12	1:A:107:THR:N	2.33	0.42
1:A:156:SER:CB	1:A:157:PRO:HD3	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:HD1	1:A:342:TYR:C	2.23	0.42
1:A:406:TRP:CG	1:A:407:GLN:N	2.87	0.42
1:A:533:LEU:HD12	1:A:533:LEU:N	2.35	0.42
2:B:42:GLU:O	2:B:42:GLU:HG2	2.20	0.42
1:A:149:LEU:HD11	1:A:159:ILE:HG21	2.01	0.42
1:A:380:ILE:HG22	1:A:381:VAL:N	2.35	0.42
2:B:225:PRO:C	2:B:227:PHE:H	2.22	0.42
2:B:60:VAL:HG13	2:B:73:LYS:HE3	2.02	0.42
2:B:75:VAL:HG21	2:B:77:PHE:CE2	2.54	0.42
2:B:76:ASP:C	2:B:78:ARG:H	2.24	0.42
2:B:195:ILE:HD13	2:B:195:ILE:H	1.85	0.42
2:B:291:GLU:O	2:B:293:ILE:N	2.53	0.42
1:A:7:THR:HG21	1:A:121:ASP:HA	2.02	0.42
1:A:42:GLU:O	1:A:45:GLY:N	2.53	0.42
1:A:229:TRP:O	1:A:230:MET:C	2.58	0.42
1:A:108:VAL:HG21	1:A:227:PHE:CZ	2.55	0.41
1:A:159:ILE:O	1:A:162:SER:N	2.53	0.41
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.55	0.41
1:A:442:VAL:HG12	1:A:443:ASP:H	1.85	0.41
2:B:23:GLN:NE2	2:B:26:LEU:CD2	2.75	0.41
2:B:77:PHE:CE2	2:B:150:PRO:HB3	2.54	0.41
2:B:197:GLN:O	2:B:201:LYS:HE2	2.20	0.41
1:A:37:ILE:CG2	1:A:38:CYS:N	2.81	0.41
1:A:96:HIS:CE1	1:A:98:ALA:CB	3.03	0.41
1:A:102:LYS:HG2	1:A:318:TYR:HB2	2.02	0.41
1:A:374:LYS:O	1:A:378:GLU:HB2	2.21	0.41
1:A:427:TYR:CE2	1:A:509:GLN:HB3	2.54	0.41
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.86	0.41
1:A:125:ARG:NH1	1:A:147:ASN:HD22	2.18	0.41
2:B:52:PRO:C	2:B:54:ASN:H	2.23	0.41
2:B:63:ILE:CG2	2:B:64:LYS:H	2.29	0.41
2:B:200:THR:C	2:B:202:ILE:H	2.23	0.41
1:A:163:SER:O	1:A:167:ILE:HG13	2.19	0.41
1:A:182:GLN:O	1:A:182:GLN:HG3	2.18	0.41
1:A:225:PRO:HB3	1:A:236:PRO:CD	2.50	0.41
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.51	0.41
1:A:532:TYR:HE1	1:A:534:ALA:HB2	1.84	0.41
2:B:28:GLU:O	2:B:29:GLU:C	2.59	0.41
2:B:300:GLU:OE1	2:B:303:LEU:HD23	2.20	0.41
1:A:23:GLN:CD	1:A:60:VAL:H	2.24	0.41
1:A:54:ASN:O	1:A:143:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG23	1:A:91:GLN:N	2.36	0.41
1:A:132:ILE:HB	1:A:142:ILE:O	2.21	0.41
1:A:416:PHE:CE1	1:A:417:VAL:O	2.74	0.41
1:A:543:GLY:C	1:A:545:ASN:N	2.74	0.41
2:B:31:ILE:HD13	2:B:133:PRO:O	2.20	0.41
2:B:346:PHE:N	2:B:346:PHE:CD1	2.88	0.41
2:B:425:LEU:CG	2:B:426:TRP:H	2.33	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD2	1.76	0.41
1:A:99:GLY:HA2	1:A:319:TYR:HB2	2.03	0.41
1:A:149:LEU:HD11	1:A:159:ILE:CG2	2.51	0.41
1:A:203:GLU:OE1	1:A:203:GLU:HA	2.19	0.41
1:A:440:PHE:N	1:A:440:PHE:HD1	2.19	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.51	0.41
1:A:523:GLU:HA	1:A:526:ILE:HB	2.02	0.41
2:B:73:LYS:HG2	2:B:74:LEU:N	2.36	0.41
2:B:161:GLN:O	2:B:164:MET:HB3	2.20	0.41
1:A:87:PHE:CE2	1:A:155:GLY:HA3	2.56	0.41
1:A:537:PRO:O	1:A:542:ILE:HG23	2.20	0.41
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.86	0.41
1:A:104:LYS:N	1:A:192:ASP:OD1	2.54	0.41
1:A:266:TRP:CZ2	1:A:269:GLN:NE2	2.86	0.41
1:A:452:LEU:H	1:A:452:LEU:HG	1.63	0.41
2:B:31:ILE:O	2:B:31:ILE:HG22	2.20	0.41
2:B:206:ARG:O	2:B:209:LEU:HB2	2.20	0.41
2:B:337:TRP:HB2	2:B:354:TYR:HB3	2.02	0.41
2:B:367:GLN:O	2:B:371:ALA:HB2	2.21	0.41
2:B:398:TRP:C	2:B:400:THR:N	2.75	0.41
1:A:1:PRO:HD3	1:A:44:GLU:HG2	2.01	0.41
2:B:193:LEU:HB3	2:B:197:GLN:CB	2.51	0.41
1:A:8:VAL:HG13	2:B:53:GLU:CG	2.51	0.40
1:A:39:THR:O	1:A:43:LYS:HD3	2.19	0.40
1:A:379:SER:OG	1:A:387:PRO:HG3	2.20	0.40
1:A:137:ASN:O	1:A:140:PRO:HD3	2.21	0.40
1:A:291:GLU:O	1:A:291:GLU:HG3	2.20	0.40
1:A:407:GLN:HG3	2:B:393:ILE:HA	2.02	0.40
1:A:515:SER:CB	1:A:518:VAL:HG23	2.51	0.40
2:B:24:TRP:O	2:B:26:LEU:HD23	2.22	0.40
2:B:110:ASP:O	2:B:112:GLY:N	2.52	0.40
2:B:236:PRO:HA	2:B:239:TRP:CZ2	2.57	0.40
2:B:386:THR:HA	2:B:387:PRO:HD3	1.82	0.40
2:B:402:TRP:O	2:B:404:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:HB2	1:A:157:PRO:CD	2.43	0.40
1:A:246:LEU:HD11	1:A:264:LEU:HD21	2.02	0.40
1:A:411:ILE:HA	1:A:412:PRO:HD2	1.81	0.40
2:B:80:LEU:O	2:B:83:ARG:HB2	2.21	0.40
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.95	0.40
2:B:380:ILE:O	2:B:384:GLY:N	2.55	0.40
2:B:394:GLN:HB3	2:B:397:THR:CB	2.51	0.40
1:A:76:ASP:C	1:A:78:ARG:H	2.25	0.40
1:A:155:GLY:O	1:A:158:ALA:N	2.52	0.40
2:B:40:GLU:O	2:B:44:GLU:HG3	2.20	0.40
2:B:132:ILE:CG2	2:B:133:PRO:HD2	2.51	0.40
2:B:235:HIS:HD1	2:B:235:HIS:N	2.19	0.40
2:B:258:GLN:NE2	2:B:289:LEU:CD2	2.81	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	Percentiles
1	A	556/558 (100%)	407 (73%)	110 (20%)	39 (7%)	1 7
2	B	428/430 (100%)	324 (76%)	69 (16%)	35 (8%)	1 5
All	All	984/988 (100%)	731 (74%)	179 (18%)	74 (8%)	1 7

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	67	ASP
1	A	104	LYS
1	A	137	ASN
1	A	154	LYS

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Mol	Chain	Res	Type
1	A	195	ILE
1	A	220	LYS
1	A	225	PRO
1	A	242	GLN
1	A	277	ARG
1	A	538	ALA
1	A	545	ASN
2	B	14	PRO
2	B	44	GLU
2	B	85	GLN
2	B	125	ARG
2	B	153	TRP
2	B	212	TRP
2	B	244	ILE
2	B	311	LYS
2	B	317	VAL
2	B	425	LEU
1	A	153	TRP
1	A	284	ARG
1	A	286	THR
1	A	413	GLU
1	A	448	ARG
1	A	540	LYS
2	B	67	ASP
2	B	98	ALA
2	B	243	PRO
2	B	278	ALA
2	B	292	VAL
2	B	315	HIS
2	B	345	PRO
2	B	356	ARG
2	B	421	PRO
2	B	427	TYR
1	A	184	MET
1	A	217	PRO
1	A	218	ASP
1	A	240	THR
1	A	321	PRO
1	A	399	GLU
2	B	78	ARG
2	B	211	ARG
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	236	PRO
1	A	247	PRO
1	A	510	PRO
2	B	69	THR
2	B	260	LEU
2	B	316	GLY
2	B	362	THR
2	B	423	VAL
1	A	243	PRO
1	A	374	LYS
1	A	436	GLY
2	B	138	GLU
2	B	160	PHE
2	B	213	GLY
1	A	63	ILE
1	A	91	GLN
1	A	156	SER
1	A	405	TYR
1	A	465	LYS
2	B	403	THR
1	A	548	VAL
2	B	381	VAL
1	A	359	GLY
2	B	169	GLU
2	B	242	GLU
1	A	176	PRO
2	B	159	ILE

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	455/498 (91%)	362 (80%)	93 (20%)	1 4
2	B	365/391 (93%)	302 (83%)	63 (17%)	2 8
All	All	820/889 (92%)	664 (81%)	156 (19%)	1 6

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	20	LYS
1	A	28	GLU
1	A	29	GLU
1	A	37	ILE
1	A	39	THR
1	A	44	GLU
1	A	46	LYS
1	A	56	TYR
1	A	61	PHE
1	A	65	LYS
1	A	76	ASP
1	A	81	ASN
1	A	94	ILE
1	A	104	LYS
1	A	107	THR
1	A	108	VAL
1	A	111	VAL
1	A	113	ASP
1	A	126	LYS
1	A	135	ILE
1	A	143	ARG
1	A	144	TYR
1	A	146	TYR
1	A	168	LEU
1	A	175	ASN
1	A	182	GLN
1	A	187	LEU
1	A	197	GLN
1	A	210	LEU
1	A	211	ARG
1	A	214	LEU
1	A	216	THR
1	A	221	HIS
1	A	223	LYS
1	A	225	PRO
1	A	227	PHE
1	A	228	LEU
1	A	234	LEU
1	A	238	LYS
1	A	242	GLN
1	A	246	LEU

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Mol	Chain	Res	Type
1	A	252	TRP
1	A	256	ASP
1	A	270	ILE
1	A	282	LEU
1	A	290	THR
1	A	291	GLU
1	A	295	LEU
1	A	296	THR
1	A	300	GLU
1	A	308	GLU
1	A	310	LEU
1	A	312	GLU
1	A	321	PRO
1	A	325	LEU
1	A	339	TYR
1	A	342	TYR
1	A	346	PHE
1	A	348	ASN
1	A	349	LEU
1	A	350	LYS
1	A	353	LYS
1	A	357	MET
1	A	361	HIS
1	A	362	THR
1	A	364	ASP
1	A	368	LEU
1	A	379	SER
1	A	380	ILE
1	A	393	ILE
1	A	397	THR
1	A	403	THR
1	A	404	GLU
1	A	409	THR
1	A	428	GLN
1	A	431	LYS
1	A	440	PHE
1	A	450	THR
1	A	451	LYS
1	A	452	LEU
1	A	460	ASN
1	A	463	ARG
1	A	473	THR

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Mol	Chain	Res	Type
1	A	482	ILE
1	A	489	SER
1	A	497	THR
1	A	503	LEU
1	A	509	GLN
1	A	512	LYS
1	A	522	ILE
1	A	540	LYS
1	A	551	LEU
2	B	11	LYS
2	B	16	MET
2	B	26	LEU
2	B	35	VAL
2	B	37	ILE
2	B	47	ILE
2	B	50	ILE
2	B	53	GLU
2	B	59	PRO
2	B	65	LYS
2	B	67	ASP
2	B	74	LEU
2	B	86	ASP
2	B	87	PHE
2	B	92	LEU
2	B	100	LEU
2	B	104	LYS
2	B	105	SER
2	B	109	LEU
2	B	115	TYR
2	B	132	ILE
2	B	139	THR
2	B	143	ARG
2	B	146	TYR
2	B	163	SER
2	B	165	THR
2	B	166	LYS
2	B	175	ASN
2	B	189	VAL
2	B	195	ILE
2	B	201	LYS
2	B	203	GLU
2	B	207	GLN

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Mol	Chain	Res	Type
2	B	210	LEU
2	B	227	PHE
2	B	233	GLU
2	B	234	LEU
2	B	235	HIS
2	B	239	TRP
2	B	240	THR
2	B	242	GLU
2	B	253	THR
2	B	260	LEU
2	B	266	TRP
2	B	290	THR
2	B	296	THR
2	B	311	LYS
2	B	318	TYR
2	B	324	ASP
2	B	330	GLN
2	B	332	GLN
2	B	345	PRO
2	B	356	ARG
2	B	358	ARG
2	B	367	GLN
2	B	369	THR
2	B	403	THR
2	B	405	TYR
2	B	409	THR
2	B	410	TRP
2	B	414	TRP
2	B	425	LEU
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	182	GLN
1	A	197	GLN
1	A	198	HIS
1	A	265	ASN
1	A	332	GLN
1	A	460	ASN
1	A	475	GLN

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Mol	Chain	Res	Type
1	A	520	GLN
1	A	524	GLN
2	B	145	GLN
2	B	197	GLN
2	B	198	HIS
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	343	GLN
2	B	348	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	559	-	23,23,23	5.64	18 (78%)	24,32,32	1.71	4 (16%)

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	559	-	-	8/13/29/29	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	559	HBY	C1-C2	16.41	1.66	1.50
3	A	559	HBY	C9-N1	9.83	1.51	1.37
3	A	559	HBY	C13-S2	7.41	1.91	1.80
3	A	559	HBY	C3-C4	7.36	1.48	1.40
3	A	559	HBY	C2-S1	6.47	1.76	1.66
3	A	559	HBY	C1-N1	6.45	1.55	1.47
3	A	559	HBY	O1-C9	5.38	1.29	1.21
3	A	559	HBY	O2-C9	5.33	1.45	1.34
3	A	559	HBY	O3-C6	5.11	1.48	1.37
3	A	559	HBY	C2-N2	5.07	1.42	1.36
3	A	559	HBY	O2-C10	3.25	1.55	1.47
3	A	559	HBY	C5-C6	3.23	1.44	1.38
3	A	559	HBY	C7-C6	3.13	1.44	1.38
3	A	559	HBY	C8-C7	2.95	1.44	1.38
3	A	559	HBY	C4-N1	2.53	1.46	1.42
3	A	559	HBY	C13-C1	2.48	1.58	1.52
3	A	559	HBY	C3-N2	2.15	1.43	1.39
3	A	559	HBY	O3-C15	2.10	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	559	HBY	O2-C9-N1	4.73	116.34	110.81
3	A	559	HBY	C3-N2-C2	-3.88	121.34	124.74
3	A	559	HBY	C10-O2-C9	3.22	121.33	116.75
3	A	559	HBY	O1-C9-N1	-2.74	119.50	124.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	559	HBY	C2-C1-C13-S2
3	A	559	HBY	N1-C1-C13-S2

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Mol	Chain	Res	Type	Atoms
3	A	559	HBY	N1-C9-O2-C10
3	A	559	HBY	O1-C9-O2-C10
3	A	559	HBY	C11-C10-O2-C9
3	A	559	HBY	O1-C9-N1-C4
3	A	559	HBY	C12-C10-O2-C9
3	A	559	HBY	O2-C9-N1-C4

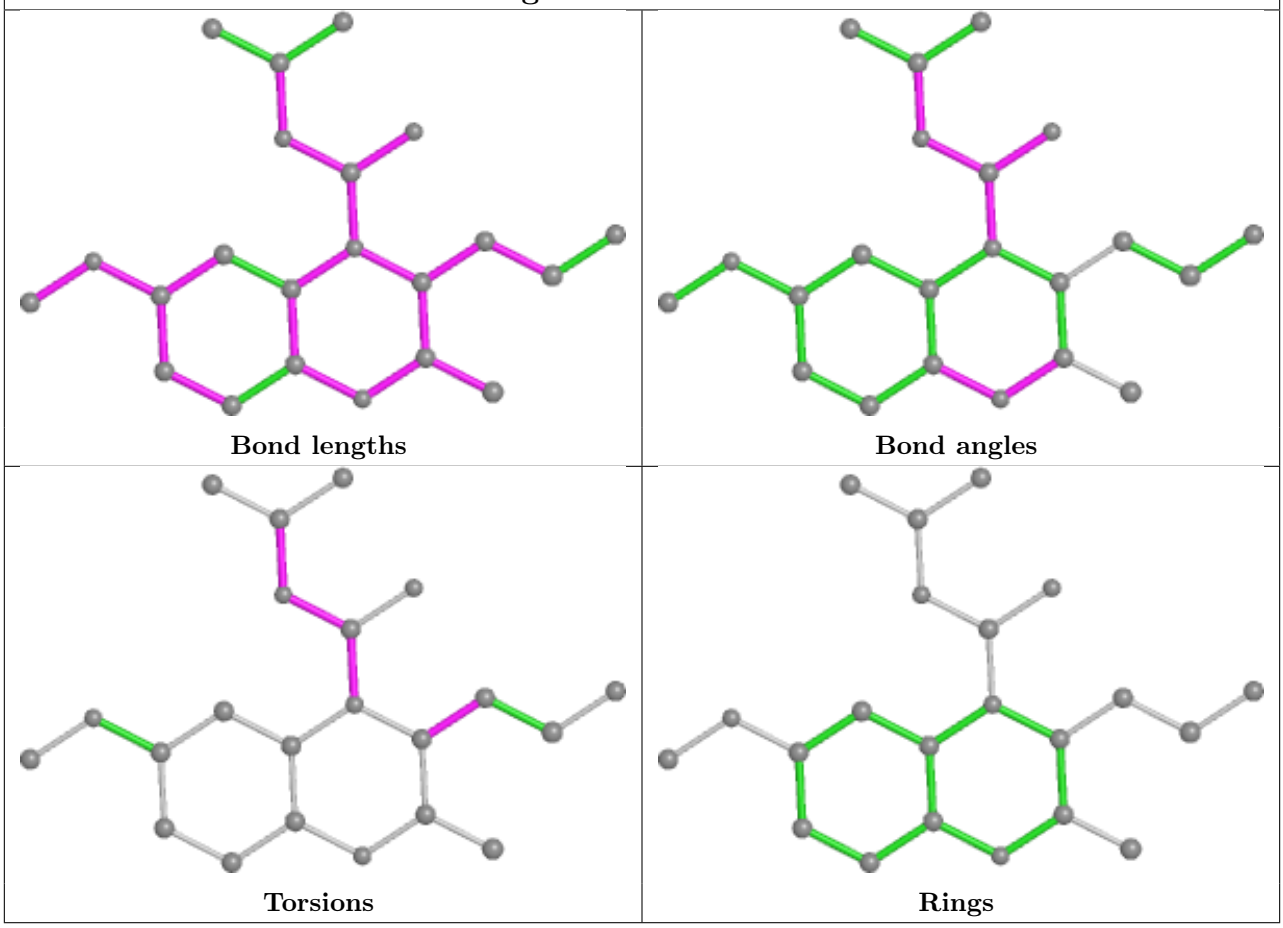
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	559	HBY	8	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 559



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.