



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:48 am BST

PDB ID : 2OPP  
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with GW420867X.  
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Deposited on : 2007-01-30  
Resolution : 2.55 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

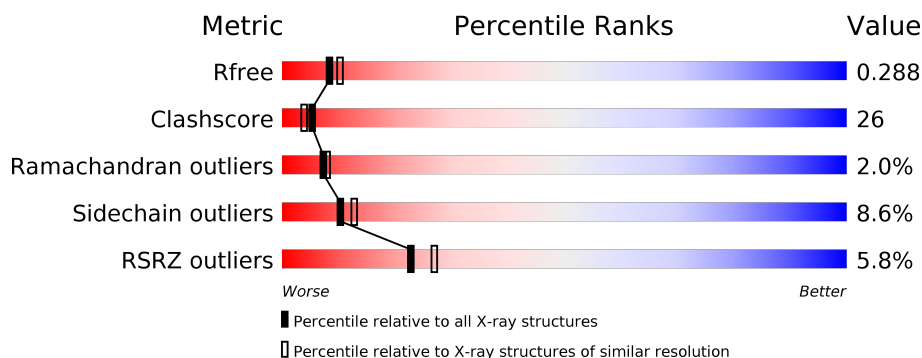
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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

Mol	Chain	Length	Quality of chain
1	A	542	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>42%</div> <div>6%</div> <div>• •</div> </div> </div>
2	B	427	<div> <div>8%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>•</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7783 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/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4261	2761	705	787	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3357	2191	552	608	6			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

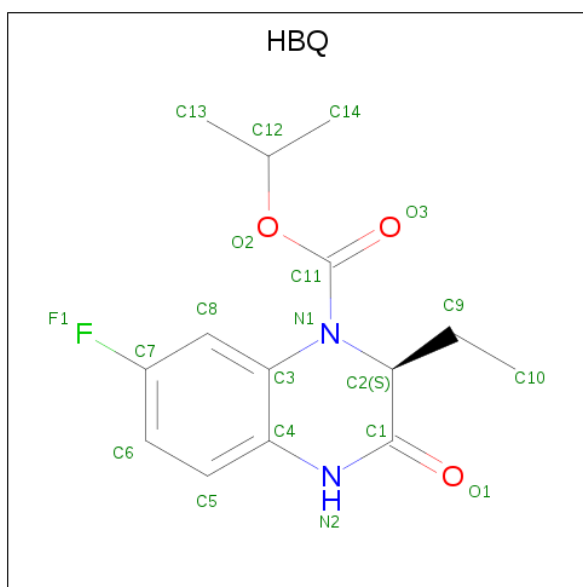


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is ISOPROPYL (2S)-2-ETHYL-7-FLUORO-3-OXO-3,4-DIHYDROQUINOXALINE-1(2H)-CARBOXYLATE (three-letter code: HBQ) (formula: C<sub>14</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C F N O 20 14 1 2 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	68	Total O 68 68	0	0
6	B	61	Total O 61 61	0	0

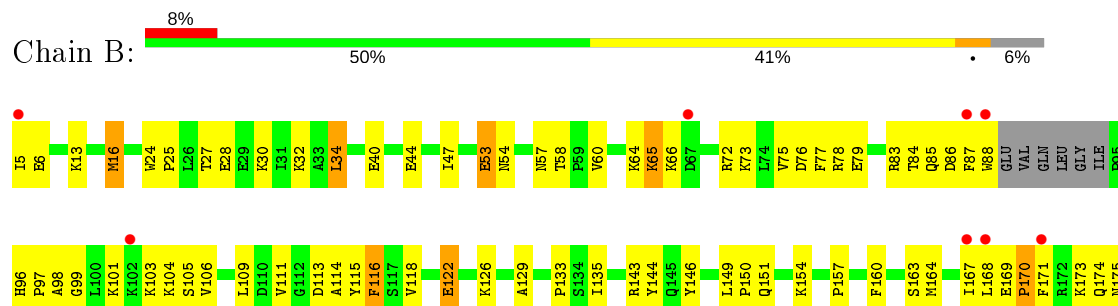
### 3 Residue-property plots

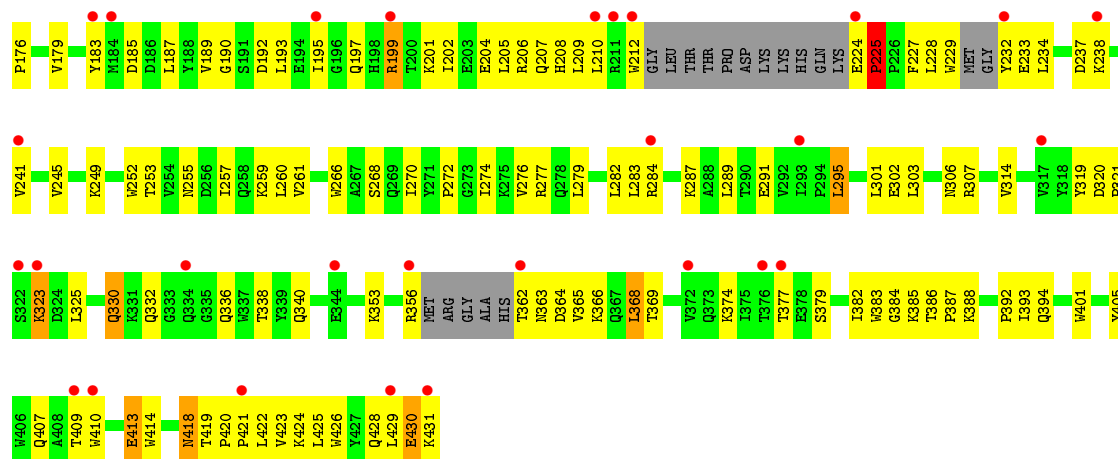
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Reverse transcriptase/ribonuclease H



#### • Molecule 2: p51 RT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.50 Å 115.30 Å 65.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.55 29.68 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.68-2.55) 94.0 (29.68-2.55)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.54 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.295 0.198 , 0.288	Depositor DCC
$R_{free}$ test set	1657 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 71.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, PO4, HBQ, MG

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	0.49	0/4366	0.70	0/5937
2	B	0.50	0/3453	0.73	1/4688 (0.0%)
All	All	0.49	0/7819	0.71	1/10625 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	234	LEU	CA-CB-CG	5.57	128.11	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	4261	0	4279	237	0
2	B	3357	0	3380	180	0
3	A	15	0	0	0	0
4	A	1	0	0	0	0
5	A	20	0	17	0	0
6	A	68	0	0	6	0
6	B	61	0	0	8	0
All	All	7783	0	7676	405	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 26.

All (405) 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:224:GLU:HB3	2:B:225:PRO:HD2	1.22	1.17
1:A:139:THR:HB	1:A:140:PRO:HD3	1.28	1.09
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.48	0.95
2:B:330:GLN:HE22	2:B:340:GLN:HE22	1.01	0.90
2:B:224:GLU:CB	2:B:225:PRO:HD2	2.03	0.89
2:B:428:GLN:HG3	2:B:429:LEU:H	1.36	0.89
1:A:22:LYS:HE3	1:A:22:LYS:HA	1.55	0.87
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.55	0.86
1:A:136:ASN:HD22	1:A:139:THR:HG23	1.41	0.85
2:B:65:LYS:HE3	2:B:66:LYS:H	1.43	0.84
1:A:46:LYS:H	1:A:46:LYS:HE2	1.42	0.83
1:A:139:THR:HB	1:A:140:PRO:CD	2.07	0.82
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.78	0.82
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.15	0.81
2:B:245:VAL:HG21	2:B:429:LEU:HD23	1.62	0.79
2:B:330:GLN:NE2	2:B:340:GLN:HE22	1.79	0.78
2:B:374:LYS:O	2:B:377:THR:HG22	1.82	0.78
1:A:91:GLN:HG3	1:A:92:LEU:H	1.46	0.78
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.18	0.78
1:A:22:LYS:CE	1:A:23:GLN:H	1.97	0.77
1:A:39:THR:O	1:A:43:LYS:HE2	1.84	0.77
2:B:224:GLU:HB3	2:B:225:PRO:CD	2.09	0.77
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.67	0.77
2:B:330:GLN:HE22	2:B:340:GLN:NE2	1.81	0.77
2:B:365:VAL:O	2:B:369:THR:HG23	1.86	0.76
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.66	0.76
1:A:376:THR:HG23	1:A:386:THR:HG22	1.68	0.76
1:A:474:ASN:O	1:A:477:THR:HG22	1.86	0.75
2:B:353:LYS:HZ1	2:B:429:LEU:HB2	1.52	0.74
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.69	0.74
1:A:286:THR:HG22	1:A:293:ILE:HD11	1.69	0.73
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.53	0.73
2:B:422:LEU:HA	2:B:425:LEU:HD13	1.71	0.73
1:A:253:THR:HG22	1:A:256:ASP:H	1.54	0.72
1:A:22:LYS:HE2	1:A:23:GLN:H	1.53	0.72
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.03	0.72
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HD11	1:A:263:LYS:NZ	2.04	0.72
1:A:518:VAL:O	1:A:522:ILE:HG13	1.89	0.72
1:A:413:GLU:HA	6:A:1063:HOH:O	1.88	0.72
2:B:169:GLU:HG2	2:B:173:LYS:NZ	2.05	0.71
2:B:209:LEU:HD13	2:B:225:PRO:HG2	1.72	0.71
1:A:301:LEU:O	1:A:305:GLU:HG3	1.92	0.70
2:B:98:ALA:HB1	2:B:101:LYS:NZ	2.06	0.70
2:B:428:GLN:CG	2:B:429:LEU:H	2.03	0.69
2:B:237:ASP:OD1	2:B:238:LYS:HG2	1.92	0.69
1:A:8:VAL:CG1	2:B:53:GLU:HG3	2.22	0.69
1:A:91:GLN:HG3	1:A:92:LEU:N	2.07	0.69
1:A:139:THR:CB	1:A:140:PRO:HD3	2.15	0.69
2:B:66:LYS:HZ1	2:B:232:TYR:N	1.91	0.69
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.28	0.69
1:A:46:LYS:N	1:A:46:LYS:HE2	2.06	0.69
1:A:54:ASN:HD22	1:A:143:ARG:NH2	1.91	0.68
2:B:431:LYS:HG2	2:B:431:LYS:OXT	1.93	0.68
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.76	0.68
2:B:72:ARG:HE	2:B:409:THR:HG22	1.59	0.68
2:B:428:GLN:CG	2:B:429:LEU:N	2.57	0.68
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.77	0.67
1:A:142:ILE:H	1:A:142:ILE:HD13	1.59	0.67
1:A:244:ILE:O	1:A:244:ILE:HG23	1.95	0.67
2:B:163:SER:O	2:B:167:ILE:HG13	1.94	0.67
2:B:66:LYS:NZ	2:B:232:TYR:N	2.43	0.67
2:B:428:GLN:HG3	2:B:429:LEU:N	2.10	0.66
1:A:136:ASN:C	1:A:138:GLU:H	1.98	0.66
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.31	0.65
2:B:353:LYS:NZ	2:B:429:LEU:HB2	2.11	0.65
1:A:197:GLN:NE2	1:A:197:GLN:HA	2.11	0.65
1:A:476:LYS:HG2	1:A:517:LEU:HD12	1.78	0.65
2:B:362:THR:HB	2:B:366:LYS:HD3	1.77	0.65
2:B:169:GLU:HG2	2:B:173:LYS:HZ2	1.59	0.65
2:B:295:LEU:HD12	2:B:295:LEU:N	2.11	0.64
1:A:218:ASP:HB2	1:A:221:HIS:ND1	2.13	0.64
2:B:224:GLU:CB	2:B:225:PRO:CD	2.73	0.64
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.80	0.64
1:A:376:THR:HG23	1:A:386:THR:CG2	2.27	0.64
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.28	0.64
2:B:5:ILE:HG23	2:B:6:GLU:H	1.62	0.64
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.33	0.63
1:A:177:ASP:O	1:A:178:ILE:HD13	1.99	0.63
1:A:275:LYS:HE2	1:A:332:GLN:NE2	2.14	0.63
2:B:287:LYS:HB3	2:B:291:GLU:OE1	1.98	0.63
1:A:275:LYS:HE2	1:A:332:GLN:CD	2.19	0.62
2:B:98:ALA:HB1	2:B:101:LYS:HZ2	1.65	0.62
1:A:111:VAL:O	1:A:111:VAL:HG23	1.99	0.62
1:A:281:LYS:O	1:A:284:ARG:HG3	2.00	0.62
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.80	0.62
1:A:503:LEU:O	1:A:507:GLN:HB2	1.99	0.62
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.82	0.62
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.30	0.62
2:B:32:LYS:HD3	6:B:1084:HOH:O	1.99	0.61
1:A:136:ASN:O	1:A:138:GLU:N	2.34	0.61
1:A:206:ARG:HH21	1:A:217:PRO:C	2.04	0.61
1:A:177:ASP:OD2	1:A:193:LEU:HD21	2.00	0.61
2:B:255:ASN:HD21	2:B:259:LYS:HE2	1.64	0.61
1:A:27:THR:HG22	1:A:30:LYS:H	1.65	0.61
2:B:199:ARG:HG2	2:B:199:ARG:HH11	1.65	0.61
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.82	0.61
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.36	0.61
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.66	0.61
1:A:206:ARG:HG2	1:A:216:THR:OG1	2.00	0.60
2:B:205:LEU:O	2:B:209:LEU:HG	2.01	0.60
1:A:210:LEU:HD21	1:A:215:THR:HG22	1.82	0.60
1:A:455:ALA:HB3	1:A:467:VAL:O	2.02	0.60
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.84	0.60
1:A:208:HIS:O	1:A:212:TRP:HD1	1.83	0.60
1:A:402:TRP:HE3	1:A:403:THR:HG1	1.47	0.60
2:B:135:ILE:HD12	2:B:135:ILE:N	2.16	0.60
1:A:545:ASN:N	1:A:545:ASN:HD22	1.99	0.59
2:B:135:ILE:H	2:B:135:ILE:HD12	1.67	0.59
1:A:139:THR:CB	1:A:140:PRO:CD	2.78	0.59
1:A:56:TYR:O	1:A:143:ARG:NH2	2.30	0.59
2:B:319:TYR:HE1	2:B:321:PRO:HG3	1.68	0.59
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.01	0.58
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.84	0.58
1:A:296:THR:HG22	1:A:298:GLU:H	1.69	0.58
2:B:64:LYS:HG2	2:B:65:LYS:N	2.18	0.58
1:A:357:MET:HE3	6:A:1042:HOH:O	2.03	0.58
1:A:281:LYS:HE3	1:A:284:ARG:CZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:HB3	1:A:139:THR:HG23	1.85	0.58
1:A:279:LEU:HA	1:A:282:LEU:HD22	1.86	0.57
1:A:201:LYS:HA	1:A:201:LYS:HE2	1.86	0.57
1:A:125:ARG:HG2	1:A:146:TYR:O	2.03	0.57
2:B:420:PRO:O	2:B:423:VAL:HG12	2.05	0.57
1:A:136:ASN:HB3	1:A:139:THR:CG2	2.35	0.57
1:A:281:LYS:HG3	1:A:284:ARG:NE	2.20	0.57
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.86	0.57
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.85	0.56
2:B:320:ASP:OD2	2:B:320:ASP:N	2.35	0.56
2:B:72:ARG:NE	2:B:409:THR:HG22	2.19	0.56
1:A:220:LYS:NZ	1:A:220:LYS:HB2	2.21	0.56
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.87	0.56
1:A:406:TRP:CH2	2:B:418:ASN:HB2	2.41	0.56
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.86	0.56
2:B:84:THR:O	2:B:154:LYS:NZ	2.29	0.56
1:A:474:ASN:O	1:A:478:GLU:HG3	2.06	0.56
2:B:53:GLU:CD	2:B:53:GLU:H	2.09	0.56
1:A:317:VAL:HG12	1:A:318:TYR:N	2.20	0.56
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.41	0.55
2:B:384:GLY:O	2:B:385:LYS:HD3	2.06	0.55
1:A:22:LYS:HE3	1:A:22:LYS:CA	2.33	0.55
1:A:44:GLU:HB3	1:A:46:LYS:HE3	1.87	0.55
2:B:174:GLN:C	2:B:176:PRO:HD3	2.27	0.55
1:A:320:ASP:OD2	1:A:323:LYS:HE2	2.06	0.55
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.36	0.55
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.89	0.55
2:B:24:TRP:CG	2:B:25:PRO:HD2	2.41	0.55
2:B:270:ILE:O	2:B:272:PRO:HD3	2.06	0.55
1:A:225:PRO:HD3	1:A:227:PHE:CZ	2.41	0.55
2:B:160:PHE:CD1	2:B:160:PHE:O	2.60	0.55
1:A:22:LYS:HE3	1:A:23:GLN:H	1.70	0.55
1:A:244:ILE:HD11	1:A:263:LYS:HZ2	1.73	0.55
1:A:244:ILE:HD11	1:A:263:LYS:HZ1	1.71	0.54
1:A:441:TYR:HB3	1:A:545:ASN:ND2	2.23	0.54
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.89	0.54
1:A:473:THR:HG22	1:A:475:GLN:H	1.72	0.54
1:A:208:HIS:O	1:A:211:ARG:HG2	2.06	0.54
1:A:78:ARG:O	1:A:82:LYS:HD3	2.08	0.54
2:B:199:ARG:HG2	2:B:199:ARG:NH1	2.22	0.54
1:A:332:GLN:HG2	1:A:332:GLN:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HA	1:A:144:TYR:O	2.08	0.53
2:B:353:LYS:HZ1	2:B:429:LEU:CB	2.21	0.53
1:A:136:ASN:C	1:A:138:GLU:N	2.62	0.53
1:A:402:TRP:CZ2	2:B:364:ASP:OD2	2.62	0.53
1:A:107:THR:HG22	1:A:109:LEU:HD13	1.91	0.53
1:A:261:VAL:O	1:A:265:ASN:OD1	2.27	0.53
1:A:344:GLU:HB3	1:A:347:LYS:HB2	1.91	0.53
1:A:44:GLU:HB3	1:A:46:LYS:CE	2.39	0.52
1:A:219:LYS:HA	1:A:222:GLN:CD	2.30	0.52
2:B:429:LEU:O	2:B:430:GLU:C	2.48	0.52
1:A:336:GLN:OE1	1:A:355:ALA:HB2	2.10	0.52
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.45	0.52
2:B:164:MET:O	2:B:168:LEU:HG	2.10	0.52
1:A:21:VAL:HG22	1:A:59:PRO:HG3	1.92	0.52
1:A:225:PRO:HA	1:A:226:PRO:C	2.30	0.51
1:A:136:ASN:ND2	1:A:139:THR:HG23	2.19	0.51
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.10	0.51
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.55	0.51
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.25	0.51
2:B:28:GLU:O	2:B:32:LYS:HB2	2.10	0.51
1:A:206:ARG:NH2	1:A:218:ASP:OD2	2.43	0.51
2:B:424:LYS:HB2	6:B:1061:HOH:O	2.10	0.51
2:B:183:TYR:OH	2:B:386:THR:HG23	2.11	0.51
2:B:58:THR:HG23	2:B:76:ASP:O	2.11	0.51
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.45	0.50
1:A:271:TYR:CE1	1:A:314:VAL:HG22	2.47	0.50
2:B:5:ILE:HG23	2:B:6:GLU:N	2.25	0.50
1:A:402:TRP:HE3	1:A:403:THR:OG1	1.95	0.50
1:A:312:GLU:HG3	1:A:312:GLU:O	2.12	0.50
2:B:106:VAL:HA	2:B:189:VAL:O	2.12	0.50
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.47	0.50
1:A:319:TYR:HA	1:A:349:LEU:HD21	1.94	0.50
2:B:116:PHE:HZ	2:B:151:GLN:HE21	1.60	0.50
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.40	0.50
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.47	0.50
1:A:27:THR:CG2	1:A:29:GLU:H	2.25	0.50
1:A:240:THR:OG1	1:A:241:VAL:N	2.45	0.50
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.38	0.50
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.24	0.49
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.93	0.49
2:B:303:LEU:O	2:B:307:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:SER:O	1:A:519:ASN:ND2	2.45	0.49
2:B:295:LEU:HD12	2:B:295:LEU:H	1.78	0.49
2:B:295:LEU:CD1	2:B:295:LEU:N	2.76	0.49
2:B:429:LEU:O	2:B:430:GLU:O	2.30	0.49
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.16	0.49
2:B:193:LEU:HD21	2:B:197:GLN:HB3	1.93	0.49
2:B:97:PRO:C	2:B:99:GLY:H	2.16	0.49
1:A:216:THR:HB	1:A:217:PRO:HD2	1.95	0.49
1:A:429:LEU:HB3	6:A:1075:HOH:O	2.12	0.49
1:A:178:ILE:HD12	1:A:191:SER:HB3	1.94	0.48
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.41	0.48
1:A:497:THR:O	1:A:535:TRP:HA	2.13	0.48
2:B:241:VAL:HG21	6:B:1173:HOH:O	2.12	0.48
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.48	0.48
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.13	0.48
2:B:79:GLU:O	2:B:83:ARG:HG3	2.13	0.48
2:B:419:THR:HG23	2:B:423:VAL:CG1	2.44	0.48
1:A:535:TRP:CH2	1:A:537:PRO:HG3	2.48	0.48
2:B:104:LYS:HD2	2:B:192:ASP:O	2.13	0.48
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.95	0.48
1:A:39:THR:O	1:A:43:LYS:CE	2.60	0.48
2:B:302:GLU:HG3	6:B:1171:HOH:O	2.12	0.48
1:A:498:ASP:HA	1:A:536:VAL:O	2.14	0.48
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.78	0.48
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.28	0.48
1:A:86:ASP:HA	1:A:154:LYS:HZ3	1.77	0.48
2:B:233:GLU:CD	2:B:233:GLU:H	2.17	0.48
1:A:21:VAL:HG22	1:A:59:PRO:CG	2.44	0.48
1:A:530:LYS:HA	6:A:1073:HOH:O	2.12	0.48
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.78	0.48
1:A:257:ILE:HD12	1:A:282:LEU:HD23	1.96	0.48
2:B:151:GLN:HG3	6:B:1006:HOH:O	2.13	0.48
1:A:340:GLN:HA	1:A:351:THR:HA	1.95	0.47
2:B:135:ILE:CD1	2:B:135:ILE:H	2.27	0.47
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.49	0.47
1:A:108:VAL:HG12	1:A:227:PHE:HE1	1.79	0.47
1:A:420:PRO:HA	1:A:421:PRO:C	2.34	0.47
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.49	0.47
1:A:21:VAL:O	1:A:57:ASN:ND2	2.48	0.47
2:B:154:LYS:O	2:B:157:PRO:HD2	2.13	0.47
1:A:211:ARG:CB	1:A:211:ARG:NH1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ARG:O	2:B:209:LEU:HB2	2.15	0.47
1:A:438:GLU:OE1	1:A:459:THR:HG21	2.15	0.47
1:A:193:LEU:CD1	1:A:201:LYS:HG3	2.45	0.47
1:A:23:GLN:NE2	1:A:24:TRP:CD1	2.83	0.47
1:A:53:GLU:O	1:A:55:PRO:HD3	2.15	0.47
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.50	0.47
1:A:545:ASN:N	1:A:545:ASN:ND2	2.63	0.47
1:A:63:ILE:N	1:A:63:ILE:HD12	2.31	0.47
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.50	0.47
2:B:13:LYS:HD2	2:B:16:MET:CE	2.45	0.46
2:B:105:SER:O	2:B:190:GLY:HA2	2.15	0.46
1:A:463:ARG:NH2	1:A:488:ASP:O	2.45	0.46
1:A:483:TYR:CZ	1:A:520:GLN:HB3	2.51	0.46
1:A:204:GLU:O	1:A:207:GLN:N	2.48	0.46
1:A:54:ASN:HD22	1:A:143:ARG:HH22	1.61	0.46
2:B:295:LEU:H	2:B:295:LEU:CD1	2.28	0.46
2:B:97:PRO:C	2:B:99:GLY:N	2.69	0.46
1:A:177:ASP:C	1:A:178:ILE:HD13	2.36	0.46
1:A:211:ARG:HB2	1:A:211:ARG:NH1	2.30	0.46
2:B:195:ILE:O	2:B:199:ARG:HD2	2.16	0.46
1:A:31:ILE:O	1:A:35:VAL:HG23	2.15	0.46
1:A:473:THR:O	1:A:475:GLN:N	2.49	0.46
1:A:91:GLN:CG	1:A:92:LEU:H	2.22	0.46
1:A:111:VAL:HG22	1:A:185:ASP:O	2.15	0.46
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.84	0.46
1:A:200:THR:O	1:A:204:GLU:HG3	2.16	0.45
1:A:441:TYR:HB3	1:A:545:ASN:HD21	1.81	0.45
2:B:279:LEU:O	2:B:282:LEU:HB2	2.16	0.45
1:A:317:VAL:HG12	1:A:318:TYR:H	1.81	0.45
2:B:118:VAL:HB	2:B:149:LEU:HG	1.97	0.45
1:A:26:LEU:HD12	1:A:133:PRO:HD2	1.99	0.45
1:A:210:LEU:C	1:A:212:TRP:H	2.20	0.45
1:A:317:VAL:HG21	1:A:347:LYS:HD3	1.99	0.45
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.52	0.45
1:A:54:ASN:O	1:A:143:ARG:NH2	2.47	0.45
2:B:173:LYS:O	2:B:176:PRO:HD3	2.17	0.45
2:B:379:SER:HA	2:B:383:TRP:CE3	2.51	0.45
1:A:347:LYS:HA	1:A:347:LYS:HE2	1.99	0.45
1:A:473:THR:O	1:A:476:LYS:N	2.50	0.45
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.52	0.45
1:A:105:SER:HB2	1:A:198:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG23	1:A:255:ASN:H	1.81	0.45
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.15	0.45
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.52	0.44
2:B:98:ALA:HB1	2:B:101:LYS:HZ1	1.80	0.44
1:A:315:HIS:HE1	1:A:347:LYS:NZ	2.15	0.44
1:A:46:LYS:HG3	1:A:148:VAL:HG21	1.98	0.44
1:A:164:MET:HG3	1:A:168:LEU:HD22	1.98	0.44
1:A:120:LEU:O	1:A:121:ASP:C	2.54	0.44
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.53	0.44
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.47	0.44
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.18	0.44
1:A:245:VAL:HG12	1:A:246:LEU:N	2.32	0.44
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.52	0.44
1:A:50:ILE:HD12	1:A:54:ASN:CB	2.48	0.44
2:B:64:LYS:HG2	2:B:65:LYS:H	1.83	0.44
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.78	0.44
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	0.44
1:A:473:THR:O	1:A:474:ASN:C	2.56	0.44
1:A:361:HIS:CE1	1:A:513:SER:HG	2.30	0.44
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.00	0.44
1:A:253:THR:HG23	1:A:289:LEU:O	2.17	0.44
1:A:407:GLN:HG2	2:B:393:ILE:HA	2.00	0.44
1:A:211:ARG:HB3	1:A:211:ARG:HH11	1.83	0.43
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.18	0.43
2:B:228:LEU:O	2:B:229:TRP:HB2	2.18	0.43
2:B:40:GLU:HG3	2:B:44:GLU:OE2	2.18	0.43
1:A:206:ARG:NE	1:A:217:PRO:O	2.48	0.43
1:A:344:GLU:O	1:A:345:PRO:C	2.55	0.43
2:B:171:PHE:CE1	2:B:205:LEU:HA	2.53	0.43
2:B:175:ASN:N	2:B:176:PRO:HD3	2.33	0.43
2:B:208:HIS:ND1	2:B:208:HIS:O	2.51	0.43
2:B:85:GLN:HA	6:B:1097:HOH:O	2.17	0.43
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.51	0.43
1:A:33:ALA:O	1:A:37:ILE:HG12	2.18	0.43
1:A:62:ALA:C	1:A:63:ILE:HD12	2.38	0.43
2:B:202:ILE:HG21	2:B:227:PHE:HE1	1.82	0.43
2:B:122:GLU:O	2:B:122:GLU:OE1	2.37	0.43
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.83	0.43
1:A:219:LYS:HD3	1:A:219:LYS:O	2.18	0.43
1:A:516:GLU:N	6:A:1071:HOH:O	2.40	0.43
1:A:97:PRO:HB2	1:A:239:TRP:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ARG:HD2	2:B:413:GLU:OE1	2.19	0.43
1:A:417:VAL:O	1:A:417:VAL:HG13	2.19	0.43
1:A:51:GLY:HA2	1:A:52:PRO:HD3	1.92	0.43
2:B:87:PHE:C	2:B:88:TRP:HD1	2.22	0.43
1:A:154:LYS:HE3	6:A:1003:HOH:O	2.19	0.43
2:B:379:SER:HB2	2:B:387:PRO:HD3	2.01	0.43
2:B:54:ASN:ND2	2:B:126:LYS:HB2	2.34	0.43
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.65	0.43
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.90	0.42
1:A:218:ASP:HB2	1:A:221:HIS:CE1	2.54	0.42
1:A:457:TYR:C	1:A:457:TYR:CD1	2.92	0.42
2:B:171:PHE:HE1	2:B:204:GLU:O	2.02	0.42
2:B:34:LEU:HD12	2:B:34:LEU:HA	1.85	0.42
1:A:281:LYS:HE3	1:A:284:ARG:NH2	2.34	0.42
2:B:206:ARG:HD2	2:B:225:PRO:O	2.19	0.42
2:B:320:ASP:OD1	2:B:323:LYS:HE2	2.19	0.42
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.54	0.42
2:B:366:LYS:HA	2:B:405:TYR:CD1	2.54	0.42
2:B:65:LYS:CE	2:B:66:LYS:H	2.23	0.42
1:A:27:THR:HG23	1:A:29:GLU:H	1.82	0.42
1:A:358:ARG:HG3	1:A:370:GLU:OE2	2.19	0.42
2:B:175:ASN:ND2	2:B:201:LYS:CE	2.82	0.42
2:B:210:LEU:HD22	2:B:224:GLU:HB2	2.01	0.42
1:A:41:MET:HB3	1:A:47:ILE:HG12	2.00	0.42
2:B:353:LYS:NZ	2:B:428:GLN:HG3	2.34	0.42
1:A:347:LYS:CE	1:A:347:LYS:HA	2.50	0.42
2:B:103:LYS:HE3	2:B:179:VAL:HG21	2.02	0.42
1:A:8:VAL:HG13	2:B:53:GLU:HG3	1.98	0.42
1:A:505:ILE:O	1:A:510:PRO:HD3	2.19	0.42
2:B:421:PRO:O	2:B:425:LEU:HD13	2.20	0.42
1:A:108:VAL:CG1	1:A:227:PHE:CE1	3.03	0.42
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.50	0.42
2:B:332:GLN:CG	2:B:338:THR:HG23	2.49	0.42
1:A:9:PRO:O	2:B:53:GLU:HG2	2.20	0.42
1:A:136:ASN:HB3	1:A:139:THR:OG1	2.19	0.42
2:B:129:ALA:HA	2:B:144:TYR:O	2.19	0.42
2:B:65:LYS:NZ	2:B:227:PHE:O	2.52	0.42
1:A:220:LYS:HZ2	1:A:220:LYS:HB2	1.84	0.42
1:A:29:GLU:CD	1:A:71:TRP:HH2	2.22	0.42
1:A:406:TRP:HH2	2:B:418:ASN:HB2	1.81	0.42
1:A:503:LEU:HD11	1:A:507:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:LEU:HB3	6:B:1170:HOH:O	2.20	0.42
1:A:91:GLN:CG	1:A:92:LEU:N	2.78	0.41
1:A:126:LYS:NZ	1:A:127:TYR:CZ	2.88	0.41
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.54	0.41
1:A:246:LEU:HD22	1:A:260:LEU:HD11	2.03	0.41
2:B:382:ILE:HG22	2:B:383:TRP:CE2	2.55	0.41
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.51	0.41
1:A:170:PRO:O	1:A:173:LYS:N	2.51	0.41
1:A:411:ILE:HG22	1:A:412:PRO:O	2.21	0.41
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.85	0.41
2:B:253:THR:O	2:B:257:ILE:HG12	2.20	0.41
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.91	0.41
1:A:296:THR:HG22	1:A:297:GLU:N	2.35	0.41
1:A:211:ARG:CB	1:A:211:ARG:HH11	2.33	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.78	0.41
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.86	0.41
1:A:59:PRO:C	1:A:60:VAL:HG23	2.41	0.41
2:B:13:LYS:HD2	2:B:16:MET:HE2	2.02	0.41
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.39	0.41
2:B:111:VAL:HG12	2:B:225:PRO:HG3	2.03	0.41
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.53	0.41
2:B:229:TRP:CZ2	2:B:377:THR:HG21	2.56	0.41
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.56	0.41
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.56	0.41
2:B:167:ILE:HG23	2:B:212:TRP:CD2	2.55	0.40
2:B:16:MET:HE3	2:B:83:ARG:HA	2.03	0.40
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.56	0.40
2:B:419:THR:HG23	2:B:423:VAL:HG11	2.03	0.40
1:A:167:ILE:HG22	1:A:167:ILE:O	2.21	0.40
1:A:469:LEU:CD1	1:A:480:GLN:HG3	2.51	0.40
2:B:307:ARG:NH1	6:B:1106:HOH:O	2.52	0.40
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.57	0.40
2:B:319:TYR:CD1	2:B:319:TYR:C	2.93	0.40
1:A:26:LEU:HB2	1:A:133:PRO:HG3	2.04	0.40
1:A:94:ILE:HD13	1:A:230:MET:HG3	2.02	0.40
1:A:358:ARG:NH2	2:B:394:GLN:CG	2.84	0.40
1:A:400:THR:O	1:A:404:GLU:HG2	2.21	0.40
1:A:51:GLY:O	1:A:53:GLU:N	2.49	0.40
2:B:146:TYR:CE2	2:B:150:PRO:HB3	2.56	0.40
2:B:332:GLN:HB2	2:B:336:GLN:O	2.22	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	511/542 (94%)	469 (92%)	31 (6%)	11 (2%)	6	7
2	B	393/427 (92%)	360 (92%)	26 (7%)	7 (2%)	8	10
All	All	904/969 (93%)	829 (92%)	57 (6%)	18 (2%)	7	8

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	139	THR
1	A	140	PRO
2	B	225	PRO
2	B	430	GLU
1	A	138	GLU
2	B	277	ARG
1	A	195	ILE
1	A	418	ASN
1	A	474	ASN
2	B	116	PHE
1	A	244	ILE
1	A	345	PRO
2	B	170	PRO
2	B	284	ARG
1	A	52	PRO
1	A	18	GLY
2	B	392	PRO

### 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	467/483 (97%)	424 (91%)	43 (9%)	9	11
2	B	370/389 (95%)	341 (92%)	29 (8%)	12	16
All	All	837/872 (96%)	765 (91%)	72 (9%)	10	13

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	21	VAL
1	A	22	LYS
1	A	27	THR
1	A	43	LYS
1	A	44	GLU
1	A	46	LYS
1	A	53	GLU
1	A	61	PHE
1	A	71	TRP
1	A	104	LYS
1	A	122	GLU
1	A	134	SER
1	A	138	GLU
1	A	139	THR
1	A	142	ILE
1	A	168	LEU
1	A	206	ARG
1	A	253	THR
1	A	264	LEU
1	A	282	LEU
1	A	314	VAL
1	A	336	GLN
1	A	340	GLN
1	A	345	PRO
1	A	347	LYS
1	A	353	LYS
1	A	358	ARG
1	A	362	THR
1	A	374	LYS
1	A	388	LYS

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Mol	Chain	Res	Type
1	A	395	LYS
1	A	418	ASN
1	A	443	ASP
1	A	479	LEU
1	A	480	GLN
1	A	484	LEU
1	A	507	GLN
1	A	516	GLU
1	A	517	LEU
1	A	533	LEU
2	B	16	MET
2	B	34	LEU
2	B	53	GLU
2	B	60	VAL
2	B	65	LYS
2	B	86	ASP
2	B	109	LEU
2	B	113	ASP
2	B	122	GLU
2	B	133	PRO
2	B	199	ARG
2	B	207	GLN
2	B	225	PRO
2	B	249	LYS
2	B	268	SER
2	B	283	LEU
2	B	289	LEU
2	B	295	LEU
2	B	314	VAL
2	B	323	LYS
2	B	330	GLN
2	B	356	ARG
2	B	368	LEU
2	B	388	LYS
2	B	407	GLN
2	B	410	TRP
2	B	413	GLU
2	B	414	TRP
2	B	418	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	136	ASN
1	A	137	ASN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	235	HIS
1	A	265	ASN
1	A	278	GLN
1	A	315	HIS
1	A	418	ASN
1	A	475	GLN
1	A	480	GLN
1	A	507	GLN
1	A	509	GLN
1	A	520	GLN
1	A	524	GLN
1	A	545	ASN
2	B	57	ASN
2	B	147	ASN
2	B	175	ASN
2	B	255	ASN
2	B	278	GLN
2	B	330	GLN
2	B	336	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
1	CSD	A	280	1	3,7,8	0.56	0	1,8,10	6.98	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	280	CSD	OD1-SG-CB	6.98	118.82	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	PO4	A	1301	-	4,4,4	1.69	0	6,6,6	0.42	0
3	PO4	A	1302	-	4,4,4	1.54	0	6,6,6	0.44	0
3	PO4	A	1300	-	4,4,4	1.67	0	6,6,6	0.44	0
5	HBQ	A	999	-	21,21,21	1.39	2 (9%)	28,30,30	1.14	2 (7%)

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
5	HBQ	A	999	-	-	0/10/26/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	HBQ	C3-N1	3.24	1.47	1.42
5	A	999	HBQ	C11-N1	3.04	1.41	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	HBQ	O2-C11-N1	2.83	114.12	110.81
5	A	999	HBQ	O3-C11-N1	-2.62	119.70	124.09

There are no chirality outliers.

There are no torsion outliers.

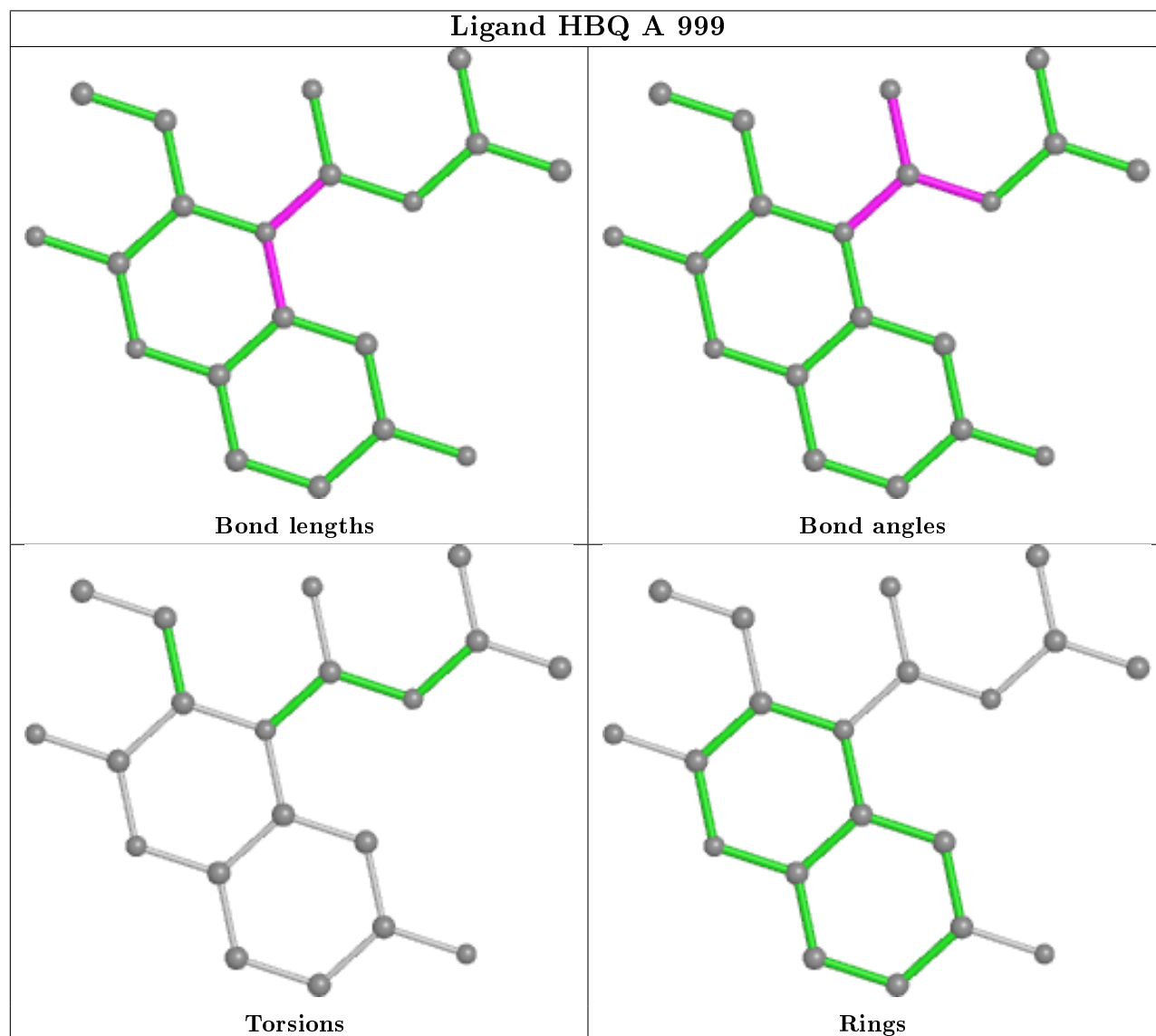
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the



average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	518/542 (95%)	-0.09	17 (3%) 46 53	29, 59, 104, 137	0
2	B	403/427 (94%)	0.19	36 (8%) 9 11	29, 58, 108, 125	0
All	All	921/969 (95%)	0.03	53 (5%) 23 27	29, 59, 105, 137	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	431	LYS	4.7
1	A	245	VAL	4.7
2	B	195	ILE	4.5
2	B	88	TRP	4.5
1	A	14	PRO	4.4
1	A	402	TRP	4.3
2	B	211	ARG	3.9
1	A	539	HIS	3.8
1	A	243	PRO	3.7
2	B	232	TYR	3.5
1	A	538	ALA	3.4
1	A	137	ASN	3.4
1	A	469	LEU	3.2
2	B	168	LEU	3.2
1	A	311	LYS	3.2
2	B	429	LEU	3.2
2	B	67	ASP	3.0
2	B	362	THR	2.9
1	A	71	TRP	2.8
1	A	52	PRO	2.8
2	B	167	ILE	2.8
2	B	184	MET	2.8
2	B	212	TRP	2.7
2	B	87	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	34	LEU	2.7
1	A	139	THR	2.6
2	B	356	ARG	2.6
2	B	183	TYR	2.6
1	A	468	THR	2.6
2	B	322	SER	2.6
2	B	376	THR	2.5
2	B	377	THR	2.5
2	B	317	VAL	2.4
1	A	403	THR	2.4
2	B	171	PHE	2.4
2	B	241	VAL	2.4
2	B	409	THR	2.3
2	B	5	ILE	2.3
2	B	410	TRP	2.3
2	B	334	GLN	2.2
2	B	344	GLU	2.2
2	B	199	ARG	2.2
2	B	293	ILE	2.2
2	B	210	LEU	2.2
2	B	284	ARG	2.2
2	B	323	LYS	2.2
2	B	238	LYS	2.2
2	B	421	PRO	2.2
2	B	224	GLU	2.2
1	A	244	ILE	2.1
2	B	102	LYS	2.1
2	B	372	VAL	2.1
1	A	138	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSD	A	280	8/9	0.96	0.11	42,56,89,100	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

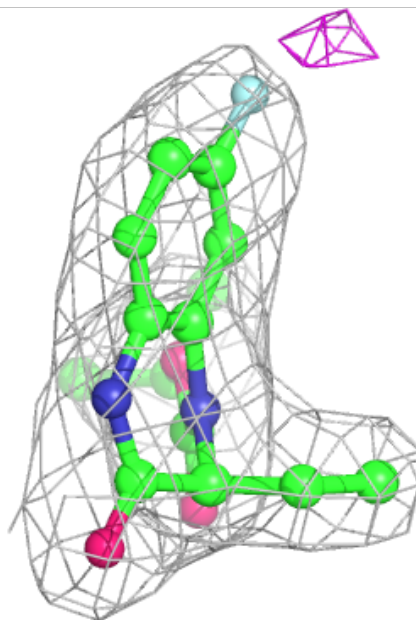
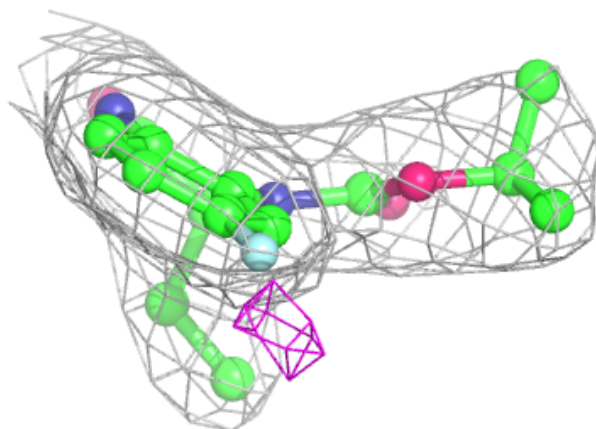
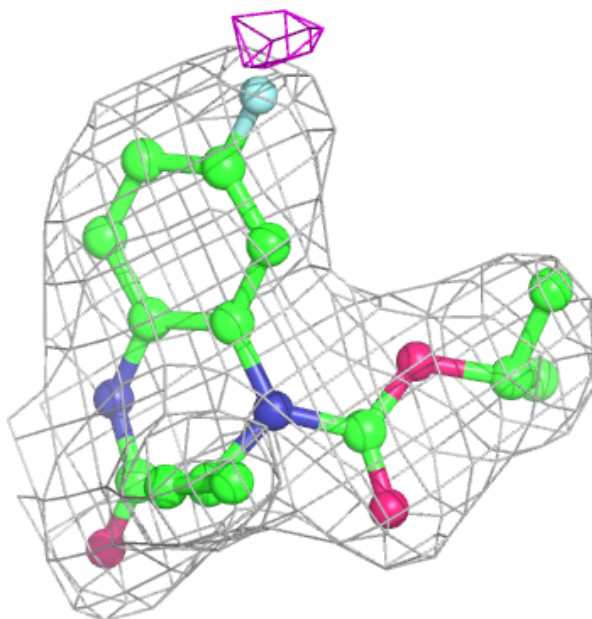
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	1302	5/5	0.86	0.17	122,123,133,136	0
3	PO4	A	1300	5/5	0.90	0.17	115,118,125,138	0
3	PO4	A	1301	5/5	0.95	0.11	91,113,117,118	0
4	MG	A	1303	1/1	0.96	0.20	66,66,66,66	0
5	HBQ	A	999	20/20	0.98	0.12	19,35,49,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around HBQ A 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.