



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:09 am BST

PDB ID : 1RT2  
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE COM-  
PLEXED WITH TNK-651  
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D.; Stuart, D.  
Deposited on : 1996-03-16  
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) : **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) : 2.11

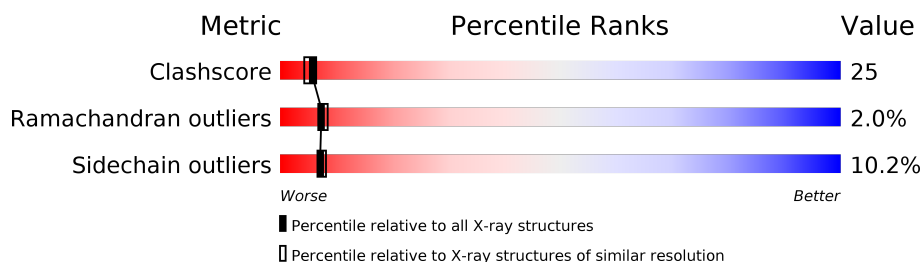
# 1 Overall quality at a glance

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))
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7934 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4435	2869	739	819	8			

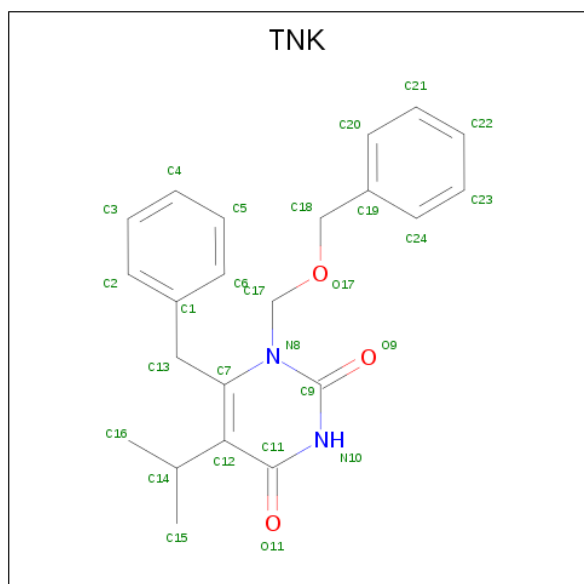
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3334	2165	554	608	7			

- Molecule 3 is 6-BENZYL-1-BENZYLOXYMETHYL-5-ISOPROPYL URACIL (three-letter code: TNK) (formula:  $C_{22}H_{24}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	2	3		

- Molecule 4 is water.

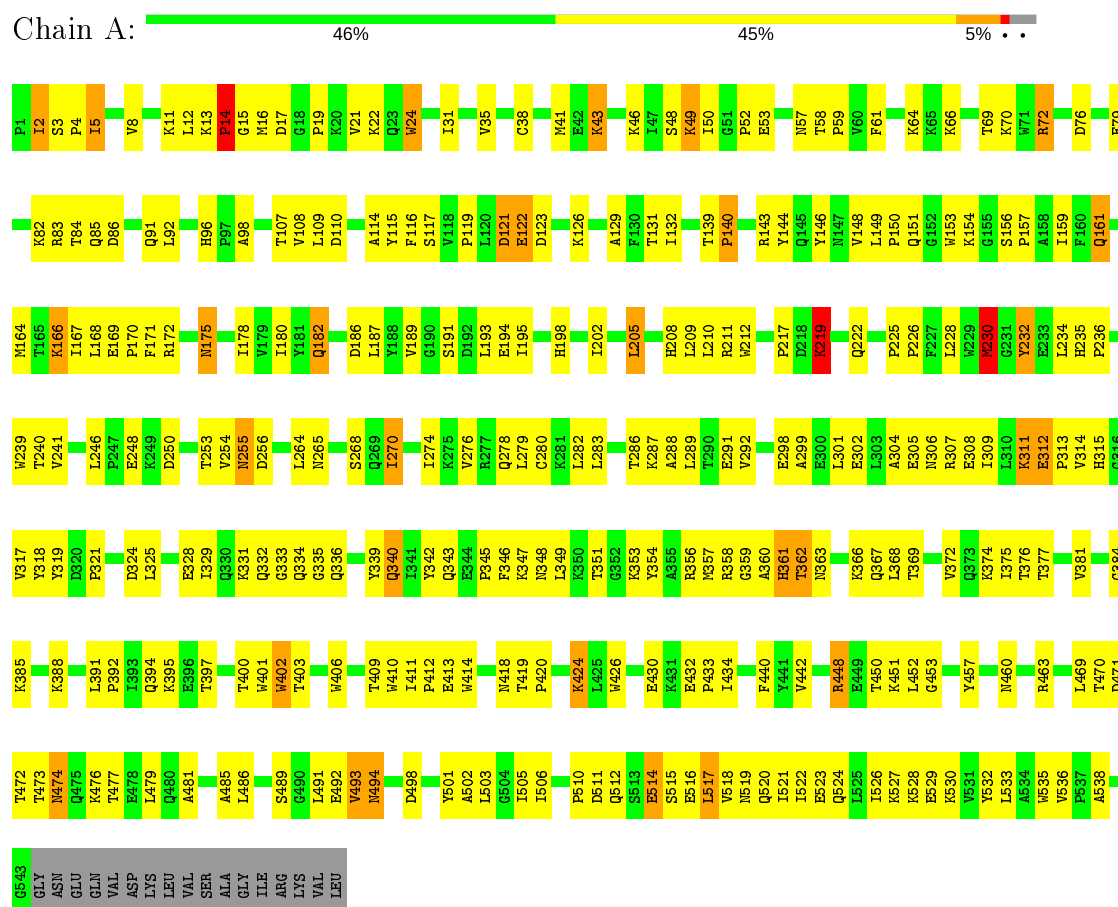
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total	O	0	0
			88	88		
4	B	50	Total	O	0	0
			50	50		

### 3 Residue-property plots

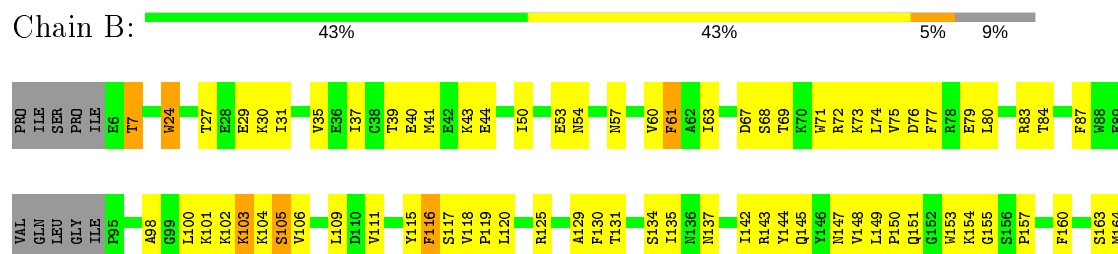
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: HIV-1 REVERSE TRANSCRIPTASE



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



K394	K395	E396	T397	W398	E399	T400	W401	W402	W406	I411	P412	E413	N418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	Q428	E432	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE																				
I325	I326	A327	E328	I329	Q330	K331	Q332	G333	Q334	G335	Q336	K337	T338	I341	Y342	G343	E344	K347	N348	I349	K350	T351	Y354	M357	K358	G359	A360	R361	T362	V365	K366	Q367	L368	T369	E370	A371	V372	Q373	K374	I375	T376	T377	I382	W383	T386	P387	K388	F389	K390	I393		
E233	L234	H235	P236	D237	K238	W239	T240	V241	Q242	P243	L244	E248	K249	D250	S251	W252	T253	V254	N255	D256	I257	Q258	K259	L260	W266	A267	S268	Q269	I270	Y271	P272	V276	R277	Q278	L283	A288	L289	E298	A299	E300	L303	R307	E308	K311	E312	P313	V314	H315	G316	V317		
I167	L168	E169	P170	K173	Q174	V179	I180	Y181	M184	L187	Y188	V189	G190	S191	D192	L193	E194	I195	G196	Q197	H198	R199	I202	E203	E204	L205	R206	Q207	E208	L209	L210	R211	TRP	GLY	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU	PRO	PHE	LEU	TRP	MET	GLY	Y232

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.30 Å 110.20 Å 72.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55	Depositor
% Data completeness (in resolution range)	85.3 (20.00-2.55)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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: CSD, TNK

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	0.52	0/4544	0.74	3/6175 (0.0%)
2	B	0.51	0/3426	0.74	1/4649 (0.0%)
All	All	0.52	0/7970	0.74	4/10824 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	494	ASN	N-CA-C	-5.63	95.79	111.00
2	B	68	SER	N-CA-C	-5.49	96.17	111.00
1	A	388	LYS	N-CA-C	-5.20	96.97	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4435	0	4483	240	0
2	B	3334	0	3360	165	0
3	A	27	0	24	2	0
4	A	88	0	0	6	0
4	B	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7934	0	7867	392	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.

All (392) 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:328:GLU:HB3	2:B:390:LYS:HD3	1.48	0.94
1:A:241:VAL:HB	1:A:314:VAL:HG23	1.55	0.89
2:B:241:VAL:HG22	2:B:350:LYS:HG3	1.56	0.86
2:B:103:LYS:HA	2:B:103:LYS:HE3	1.58	0.85
1:A:491:LEU:HD12	1:A:529:GLU:HG3	1.60	0.83
1:A:270:ILE:HD11	1:A:314:VAL:HB	1.60	0.83
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.60	0.82
2:B:241:VAL:HG13	2:B:351:THR:H	1.42	0.82
1:A:115:TYR:HD2	1:A:156:SER:HB3	1.46	0.81
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.47	0.80
2:B:84:THR:HB	2:B:154:LYS:HE2	1.64	0.80
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.62	0.79
1:A:43:LYS:HE3	1:A:43:LYS:HA	1.65	0.78
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.65	0.77
2:B:193:LEU:HB3	2:B:197:GLN:HB3	1.68	0.76
1:A:116:PHE:CE2	1:A:151:GLN:HG3	2.20	0.76
2:B:241:VAL:HG13	2:B:351:THR:N	2.02	0.75
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.52	0.74
1:A:49:LYS:HA	1:A:143:ARG:O	1.88	0.72
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.70	0.72
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.72	0.72
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.72	0.70
1:A:402:TRP:CH2	2:B:362:THR:HA	2.26	0.70
1:A:19:PRO:HD3	1:A:83:ARG:HD2	1.74	0.70
1:A:8:VAL:O	1:A:121:ASP:HB2	1.91	0.69
2:B:24:TRP:NE1	2:B:61:PHE:HE2	1.90	0.69
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.76	0.68
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.28	0.68
1:A:278:GLN:O	1:A:282:LEU:HD13	1.94	0.68
1:A:395:LYS:HG2	1:A:414:TRP:CH2	2.27	0.68
2:B:7:THR:HG21	2:B:119:PRO:O	1.93	0.68
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.29	0.68
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.29	0.67
1:A:115:TYR:O	1:A:149:LEU:HB2	1.96	0.66
2:B:376:THR:HG23	2:B:387:PRO:HD2	1.77	0.66
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.78	0.66
1:A:450:THR:HB	1:A:452:LEU:HD23	1.76	0.66
2:B:368:LEU:O	2:B:372:VAL:HG23	1.96	0.66
1:A:426:TRP:HB3	1:A:526:ILE:HD13	1.78	0.65
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.78	0.65
1:A:168:LEU:O	1:A:172:ARG:HG3	1.97	0.64
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.96	0.64
1:A:57:ASN:HA	1:A:129:ALA:O	1.98	0.64
2:B:105:SER:HA	2:B:234:LEU:O	1.96	0.64
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.79	0.64
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.13	0.63
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.81	0.63
2:B:398:TRP:O	2:B:402:TRP:HD1	1.81	0.63
1:A:24:TRP:CE3	1:A:61:PHE:HZ	2.16	0.63
1:A:232:TYR:HB3	1:A:240:THR:O	1.99	0.63
2:B:328:GLU:HB2	2:B:390:LYS:HB2	1.81	0.63
1:A:219:LYS:HD3	1:A:222:GLN:HG3	1.81	0.62
1:A:331:LYS:HE2	1:A:333:GLY:O	2.00	0.62
1:A:24:TRP:HE3	1:A:61:PHE:HZ	1.48	0.62
2:B:103:LYS:HE2	2:B:192:ASP:HB3	1.81	0.62
2:B:40:GLU:O	2:B:44:GLU:HG3	1.99	0.62
1:A:149:LEU:HD11	1:A:159:ILE:HG22	1.82	0.62
2:B:106:VAL:HA	2:B:189:VAL:O	2.00	0.62
2:B:360:ALA:HA	2:B:366:LYS:HD3	1.82	0.61
1:A:376:THR:HG21	2:B:401:TRP:HZ2	1.65	0.61
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.35	0.61
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.35	0.61
2:B:358:ARG:HD3	2:B:358:ARG:H	1.66	0.61
2:B:39:THR:O	2:B:43:LYS:HG2	1.99	0.61
2:B:116:PHE:HD1	2:B:117:SER:N	1.98	0.61
2:B:374:LYS:NZ	2:B:374:LYS:HB2	2.15	0.61
1:A:110:ASP:HB3	1:A:217:PRO:HB3	1.82	0.61
2:B:395:LYS:O	2:B:399:GLU:HG3	2.01	0.60
1:A:517:LEU:O	1:A:521:ILE:HG13	2.01	0.60
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.60
2:B:232:TYR:HD1	2:B:233:GLU:H	1.48	0.60
2:B:232:TYR:HD1	2:B:233:GLU:N	2.00	0.60
2:B:27:THR:HG22	2:B:29:GLU:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLU:CB	2:B:390:LYS:HB2	2.32	0.59
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.84	0.59
1:A:191:SER:HG	1:A:198:HIS:HD1	1.49	0.59
2:B:337:TRP:HB2	2:B:354:TYR:HB3	1.83	0.59
2:B:101:LYS:HD2	2:B:382:ILE:HG23	1.84	0.59
2:B:195:ILE:HG23	2:B:196:GLY:H	1.68	0.58
2:B:30:LYS:NZ	2:B:71:TRP:HZ3	2.01	0.58
2:B:24:TRP:HE1	2:B:61:PHE:HE2	1.51	0.58
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.84	0.58
2:B:193:LEU:HB3	2:B:197:GLN:CB	2.33	0.58
1:A:182:GLN:HG2	1:A:187:LEU:HD23	1.85	0.57
1:A:246:LEU:HD23	1:A:307:ARG:HG2	1.86	0.57
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.34	0.57
1:A:157:PRO:O	1:A:161:GLN:HB2	2.05	0.57
1:A:5:ILE:HD13	1:A:167:ILE:HD11	1.87	0.57
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.86	0.57
2:B:169:GLU:O	2:B:173:LYS:HD3	2.05	0.57
1:A:453:GLY:HA3	1:A:472:THR:CG2	2.35	0.57
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.35	0.56
2:B:160:PHE:O	2:B:164:MET:HB2	2.05	0.56
1:A:264:LEU:HD12	1:A:274:ILE:HG23	1.87	0.56
1:A:517:LEU:HA	1:A:520:GLN:OE1	2.05	0.56
2:B:142:ILE:HG22	2:B:144:TYR:CE2	2.39	0.56
2:B:308:GLU:O	2:B:311:LYS:HB2	2.05	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.40	0.56
2:B:270:ILE:O	2:B:272:PRO:HD3	2.05	0.56
1:A:419:THR:HG21	4:A:1062:HOH:O	2.05	0.56
2:B:360:ALA:HB1	2:B:367:GLN:HG3	1.88	0.56
1:A:167:ILE:HG23	1:A:212:TRP:CD1	2.41	0.56
2:B:167:ILE:O	2:B:208:HIS:HE1	1.89	0.56
1:A:402:TRP:CH2	2:B:362:THR:HG23	2.41	0.56
1:A:12:LEU:O	1:A:13:LYS:C	2.45	0.55
1:A:239:TRP:O	1:A:315:HIS:HB2	2.06	0.55
1:A:306:ASN:HA	1:A:309:ILE:HG22	1.89	0.55
2:B:27:THR:CG2	2:B:29:GLU:HG2	2.36	0.55
2:B:79:GLU:O	2:B:83:ARG:HG3	2.05	0.55
1:A:248:GLU:HB2	4:A:1046:HOH:O	2.06	0.55
1:A:520:GLN:O	1:A:523:GLU:HB2	2.06	0.55
1:A:69:THR:HG22	1:A:69:THR:O	2.06	0.54
2:B:253:THR:O	2:B:257:ILE:HG12	2.07	0.54
2:B:373:GLN:O	2:B:377:THR:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.88	0.54
1:A:402:TRP:HH2	2:B:362:THR:HA	1.73	0.54
1:A:424:LYS:HB3	1:A:424:LYS:NZ	2.22	0.54
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.88	0.54
2:B:7:THR:HG23	2:B:119:PRO:HG2	1.90	0.54
1:A:331:LYS:CE	1:A:334:GLN:HA	2.38	0.54
2:B:317:VAL:HG22	2:B:347:LYS:HD2	1.91	0.53
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.38	0.53
2:B:154:LYS:O	2:B:157:PRO:HD2	2.08	0.53
1:A:340:GLN:HB2	1:A:351:THR:HG22	1.89	0.53
2:B:357:MET:O	2:B:359:GLY:N	2.42	0.53
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.90	0.53
1:A:514:GLU:HG3	1:A:515:SER:H	1.74	0.53
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.72	0.53
2:B:120:LEU:HB2	2:B:148:VAL:O	2.09	0.52
2:B:248:GLU:HG2	2:B:307:ARG:HH12	1.74	0.52
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.90	0.52
1:A:376:THR:HG21	2:B:401:TRP:CZ2	2.44	0.52
1:A:167:ILE:O	1:A:170:PRO:HD2	2.08	0.52
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.74	0.52
2:B:173:LYS:N	2:B:173:LYS:HD2	2.24	0.52
2:B:398:TRP:O	2:B:402:TRP:CD1	2.62	0.52
2:B:73:LYS:NZ	2:B:130:PHE:CZ	2.76	0.52
2:B:277:ARG:HG3	2:B:278:GLN:H	1.73	0.52
2:B:30:LYS:NZ	2:B:71:TRP:CZ3	2.77	0.52
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.45	0.52
1:A:70:LYS:HE3	1:A:72:ARG:NH1	2.24	0.52
2:B:366:LYS:HE2	2:B:370:GLU:OE2	2.09	0.52
1:A:2:ILE:HD12	1:A:148:VAL:CG1	2.40	0.52
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.91	0.52
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.75	0.52
1:A:523:GLU:O	1:A:527:LYS:HG2	2.10	0.51
2:B:249:LYS:HB3	2:B:252:TRP:CE2	2.46	0.51
2:B:388:LYS:HG2	2:B:413:GLU:HB3	1.91	0.51
1:A:331:LYS:HE2	1:A:334:GLN:HA	1.93	0.51
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.92	0.51
1:A:498:ASP:HA	1:A:536:VAL:O	2.10	0.51
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.46	0.51
2:B:142:ILE:HD12	2:B:142:ILE:N	2.26	0.51
1:A:479:LEU:HB3	1:A:521:ILE:HD11	1.93	0.51
2:B:266:TRP:CZ2	2:B:423:VAL:HG22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG13	2:B:53:GLU:OE1	2.11	0.51
1:A:360:ALA:HA	1:A:514:GLU:HB3	1.92	0.50
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.93	0.50
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.47	0.50
2:B:142:ILE:HD12	2:B:142:ILE:H	1.75	0.50
1:A:178:ILE:HD11	1:A:193:LEU:HD11	1.93	0.50
1:A:57:ASN:HB2	1:A:143:ARG:NH2	2.22	0.50
1:A:301:LEU:O	1:A:304:ALA:HB3	2.12	0.50
1:A:361:HIS:HB2	1:A:510:PRO:HB3	1.93	0.50
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.94	0.50
1:A:276:VAL:O	1:A:280:CSD:HB3	2.12	0.49
1:A:519:ASN:O	1:A:523:GLU:HG2	2.12	0.49
2:B:314:VAL:HG22	2:B:315:HIS:O	2.12	0.49
2:B:317:VAL:HG13	2:B:347:LYS:HB3	1.94	0.49
1:A:182:GLN:HG2	1:A:187:LEU:CD2	2.42	0.49
1:A:254:VAL:HB	1:A:289:LEU:HA	1.94	0.49
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.94	0.49
1:A:311:LYS:HE3	1:A:311:LYS:O	2.12	0.49
1:A:418:ASN:O	1:A:420:PRO:HD3	2.12	0.49
2:B:372:VAL:O	2:B:376:THR:OG1	2.28	0.49
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.48	0.49
1:A:228:LEU:N	1:A:228:LEU:HD12	2.28	0.49
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.94	0.49
1:A:361:HIS:HA	1:A:512:GLN:O	2.13	0.49
1:A:369:THR:HG21	1:A:409:THR:OG1	2.13	0.49
1:A:514:GLU:HG3	1:A:515:SER:N	2.28	0.49
2:B:103:LYS:O	2:B:236:PRO:HD2	2.12	0.49
1:A:448:ARG:HE	1:A:474:ASN:HB2	1.78	0.48
2:B:374:LYS:HZ3	2:B:374:LYS:HB2	1.76	0.48
2:B:76:ASP:HA	2:B:411:ILE:HD12	1.95	0.48
1:A:253:THR:O	1:A:256:ASP:HB2	2.13	0.48
1:A:287:LYS:HG2	1:A:291:GLU:CD	2.33	0.48
1:A:79:GLU:OE2	1:A:82:LYS:HD3	2.13	0.48
1:A:450:THR:HB	1:A:452:LEU:CD2	2.43	0.48
2:B:327:ALA:O	2:B:389:PHE:HA	2.13	0.48
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.96	0.48
1:A:430:GLU:HG2	4:A:1068:HOH:O	2.14	0.48
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.78	0.48
1:A:178:ILE:HD11	1:A:193:LEU:CD1	2.44	0.48
2:B:150:PRO:HD2	2:B:153:TRP:CE3	2.49	0.48
2:B:205:LEU:O	2:B:208:HIS:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.95	0.48
1:A:79:GLU:HA	1:A:82:LYS:HG2	1.96	0.48
1:A:384:GLY:CA	2:B:135:ILE:HD12	2.44	0.48
1:A:279:LEU:HD23	1:A:302:GLU:OE2	2.13	0.48
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.79	0.48
1:A:278:GLN:HG2	1:A:299:ALA:N	2.28	0.48
1:A:502:ALA:HA	1:A:505:ILE:HD12	1.94	0.48
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.49	0.47
1:A:535:TRP:CZ3	2:B:422:LEU:HD21	2.49	0.47
2:B:116:PHE:HD1	2:B:117:SER:HG	1.62	0.47
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.44	0.47
1:A:516:GLU:O	1:A:520:GLN:HG3	2.15	0.47
1:A:406:TRP:CE3	2:B:419:THR:HB	2.49	0.47
1:A:448:ARG:HH21	1:A:474:ASN:HB3	1.80	0.47
1:A:270:ILE:HG13	1:A:270:ILE:O	2.13	0.47
1:A:413:GLU:HG2	4:A:1065:HOH:O	2.14	0.47
2:B:371:ALA:O	2:B:375:ILE:HG13	2.15	0.47
1:A:448:ARG:NH1	1:A:473:THR:HB	2.29	0.46
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.95	0.46
1:A:334:GLN:HG2	1:A:356:ARG:NH2	2.31	0.46
1:A:11:LYS:O	1:A:85:GLN:HB3	2.15	0.46
2:B:421:PRO:O	2:B:425:LEU:HG	2.15	0.46
2:B:103:LYS:HA	2:B:103:LYS:CE	2.40	0.46
2:B:163:SER:O	2:B:167:ILE:CG2	2.63	0.46
2:B:232:TYR:CD1	2:B:233:GLU:N	2.83	0.46
2:B:278:GLN:HE21	2:B:298:GLU:HB3	1.80	0.46
1:A:345:PRO:O	1:A:346:PHE:HB2	2.14	0.46
1:A:96:HIS:CD2	1:A:98:ALA:CB	2.97	0.46
1:A:334:GLN:HG2	1:A:356:ARG:HH21	1.80	0.46
2:B:61:PHE:CD1	2:B:74:LEU:HD23	2.51	0.46
2:B:100:LEU:HD22	2:B:181:TYR:HB2	1.98	0.46
2:B:376:THR:HG22	2:B:386:THR:HG22	1.97	0.46
1:A:306:ASN:HA	1:A:309:ILE:CG2	2.45	0.46
1:A:340:GLN:CB	1:A:351:THR:HG22	2.46	0.46
1:A:363:ASN:HD21	1:A:401:TRP:HZ2	1.64	0.46
2:B:249:LYS:HG2	2:B:251:SER:O	2.15	0.46
1:A:274:ILE:HD13	1:A:309:ILE:HD13	1.97	0.46
1:A:278:GLN:HG2	1:A:298:GLU:C	2.36	0.46
1:A:354:TYR:HE2	1:A:375:ILE:HG13	1.81	0.45
1:A:108:VAL:HG23	1:A:186:ASP:HB3	1.97	0.45
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.15	0.45
2:B:254:VAL:O	2:B:258:GLN:HG3	2.17	0.45
1:A:41:MET:CE	1:A:46:LYS:HE3	2.46	0.45
1:A:13:LYS:HA	1:A:85:GLN:HA	1.98	0.45
2:B:37:ILE:O	2:B:41:MET:HG3	2.16	0.45
1:A:12:LEU:O	1:A:14:PRO:N	2.49	0.45
1:A:328:GLU:HB3	1:A:340:GLN:OE1	2.16	0.45
1:A:48:SER:O	1:A:144:TYR:HA	2.16	0.45
1:A:301:LEU:O	1:A:305:GLU:HG3	2.16	0.45
2:B:268:SER:HA	2:B:271:TYR:O	2.16	0.45
2:B:118:VAL:HA	2:B:119:PRO:HD2	1.86	0.45
1:A:194:GLU:CD	1:A:194:GLU:H	2.20	0.45
1:A:328:GLU:O	1:A:339:TYR:HA	2.17	0.45
1:A:516:GLU:HA	1:A:519:ASN:ND2	2.32	0.45
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.50	0.45
2:B:106:VAL:CG1	2:B:188:TYR:HB3	2.47	0.45
2:B:199:ARG:O	2:B:202:ILE:HG22	2.17	0.45
1:A:360:ALA:O	1:A:361:HIS:HB3	2.17	0.45
1:A:505:ILE:HG23	1:A:510:PRO:HD2	1.98	0.45
1:A:362:THR:HG22	1:A:366:LYS:HG2	1.98	0.45
1:A:524:GLN:O	1:A:528:LYS:HG2	2.17	0.44
1:A:123:ASP:O	1:A:126:LYS:HE3	2.16	0.44
1:A:53:GLU:HG2	1:A:53:GLU:O	2.18	0.44
3:A:999:TNK:H131	3:A:999:TNK:H172	1.65	0.44
1:A:115:TYR:HB2	1:A:151:GLN:NE2	2.32	0.44
1:A:166:LYS:O	1:A:169:GLU:HB3	2.16	0.44
2:B:191:SER:OG	2:B:198:HIS:ND1	2.45	0.44
2:B:311:LYS:O	2:B:312:GLU:HG3	2.18	0.44
1:A:114:ALA:HA	1:A:117:SER:HB2	1.99	0.44
1:A:319:TYR:CE1	1:A:343:GLN:NE2	2.85	0.44
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.32	0.44
2:B:365:VAL:O	2:B:369:THR:HG23	2.18	0.44
1:A:331:LYS:HE2	1:A:333:GLY:C	2.37	0.44
1:A:377:THR:O	1:A:381:VAL:HG23	2.17	0.44
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.99	0.44
2:B:424:LYS:NZ	2:B:428:GLN:HG3	2.32	0.44
1:A:114:ALA:HA	1:A:117:SER:OG	2.18	0.44
1:A:114:ALA:HA	1:A:117:SER:CB	2.48	0.44
1:A:342:TYR:HA	1:A:349:LEU:HG	1.98	0.44
1:A:472:THR:OG1	1:A:476:LYS:HB2	2.18	0.44
1:A:511:ASP:HA	1:A:522:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:HB3	1:A:307:ARG:NH2	2.33	0.44
1:A:522:ILE:O	1:A:526:ILE:HG13	2.18	0.44
1:A:17:ASP:O	1:A:83:ARG:HD3	2.18	0.44
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.83	0.43
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.48	0.43
1:A:270:ILE:HG12	1:A:314:VAL:HG21	2.00	0.43
1:A:317:VAL:HG22	1:A:318:TYR:H	1.82	0.43
2:B:180:ILE:HA	2:B:188:TYR:O	2.18	0.43
2:B:248:GLU:HG2	2:B:307:ARG:NH1	2.34	0.43
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.52	0.43
2:B:194:GLU:O	2:B:197:GLN:HB2	2.18	0.43
1:A:16:MET:HB3	1:A:17:ASP:H	1.69	0.43
2:B:237:ASP:C	2:B:239:TRP:H	2.21	0.43
2:B:277:ARG:HG3	2:B:278:GLN:N	2.32	0.43
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.78	0.43
1:A:22:LYS:HG2	4:A:1002:HOH:O	2.18	0.43
1:A:329:ILE:O	1:A:392:PRO:HD3	2.19	0.43
1:A:41:MET:HE2	1:A:46:LYS:HE3	2.01	0.43
2:B:210:LEU:O	2:B:211:ARG:CB	2.66	0.43
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.99	0.43
1:A:503:LEU:HA	1:A:506:ILE:HD12	2.00	0.43
2:B:180:ILE:HG22	2:B:187:LEU:HG	2.01	0.43
2:B:195:ILE:HG23	2:B:196:GLY:N	2.32	0.43
1:A:119:PRO:HA	1:A:148:VAL:HA	2.01	0.42
1:A:527:LYS:HE2	1:A:527:LYS:HA	2.01	0.42
2:B:31:ILE:O	2:B:35:VAL:HG23	2.19	0.42
1:A:298:GLU:H	1:A:298:GLU:CD	2.22	0.42
1:A:332:GLN:HE22	1:A:353:LYS:NZ	2.17	0.42
2:B:205:LEU:O	2:B:209:LEU:HG	2.20	0.42
2:B:388:LYS:HG2	2:B:413:GLU:CB	2.48	0.42
1:A:319:TYR:OH	1:A:385:LYS:NZ	2.49	0.42
1:A:359:GLY:C	1:A:361:HIS:N	2.72	0.42
1:A:520:GLN:HA	1:A:523:GLU:HG2	2.00	0.42
2:B:358:ARG:HG2	2:B:358:ARG:O	2.20	0.42
1:A:107:THR:N	1:A:189:VAL:O	2.49	0.42
1:A:205:LEU:O	1:A:209:LEU:HG	2.20	0.42
1:A:426:TRP:O	1:A:526:ILE:HG23	2.20	0.42
2:B:197:GLN:NE2	2:B:197:GLN:HA	2.34	0.42
2:B:393:ILE:HD13	2:B:398:TRP:HE3	1.84	0.42
1:A:307:ARG:HD2	4:A:1048:HOH:O	2.20	0.42
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:HE1	1:A:146:TYR:HE2	1.67	0.42
1:A:432:GLU:OE1	1:A:433:PRO:HD2	2.19	0.42
2:B:111:VAL:CG1	2:B:187:LEU:HD22	2.49	0.42
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.20	0.42
1:A:434:ILE:HD12	1:A:493:VAL:O	2.19	0.42
1:A:361:HIS:HB2	1:A:510:PRO:CB	2.50	0.42
2:B:326:ILE:O	2:B:341:ILE:HA	2.19	0.42
1:A:434:ILE:HD13	1:A:530:LYS:HB3	2.02	0.41
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.55	0.41
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.50	0.41
3:A:999:TNK:O11	3:A:999:TNK:H163	2.19	0.41
2:B:103:LYS:C	2:B:105:SER:H	2.23	0.41
2:B:249:LYS:HE2	2:B:249:LYS:HB2	1.88	0.41
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.60	0.41
1:A:205:LEU:O	1:A:208:HIS:HB3	2.21	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.41
1:A:79:GLU:O	1:A:83:ARG:NH1	2.53	0.41
2:B:50:ILE:HG21	2:B:145:GLN:CB	2.49	0.41
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.03	0.41
1:A:57:ASN:HD22	1:A:143:ARG:CZ	2.33	0.41
2:B:289:LEU:HD12	2:B:289:LEU:HA	1.76	0.41
2:B:35:VAL:O	2:B:39:THR:HG23	2.21	0.41
2:B:63:ILE:CD1	2:B:74:LEU:HB2	2.50	0.41
1:A:150:PRO:HG2	1:A:153:TRP:HB2	2.03	0.41
2:B:163:SER:O	2:B:167:ILE:HG23	2.20	0.41
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.35	0.41
1:A:340:GLN:HA	1:A:351:THR:HA	2.02	0.41
1:A:79:GLU:O	1:A:83:ARG:HG2	2.20	0.41
2:B:134:SER:OG	2:B:137:ASN:HA	2.20	0.41
2:B:255:ASN:O	2:B:258:GLN:HB2	2.21	0.41
2:B:359:GLY:O	2:B:361:HIS:CD2	2.74	0.41
1:A:278:GLN:HG2	1:A:298:GLU:HB2	2.02	0.41
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.65	0.41
1:A:489:SER:HB2	1:A:493:VAL:HG13	2.02	0.41
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.35	0.41
1:A:96:HIS:CD2	1:A:98:ALA:H	2.38	0.41
2:B:344:GLU:HB3	2:B:347:LYS:HB2	2.03	0.41
1:A:319:TYR:HE1	1:A:343:GLN:NE2	2.18	0.41
1:A:84:THR:HB	1:A:154:LYS:HD3	2.03	0.41
2:B:142:ILE:CG2	2:B:144:TYR:CE2	3.02	0.41
1:A:164:MET:O	1:A:168:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ARG:O	2:B:145:GLN:HG3	2.19	0.41
2:B:181:TYR:O	2:B:187:LEU:HA	2.21	0.41
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.02	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.03	0.41
2:B:406:TRP:CH2	2:B:412:PRO:HD3	2.56	0.41
1:A:372:VAL:O	1:A:375:ILE:HB	2.21	0.41
1:A:225:PRO:HA	1:A:226:PRO:C	2.41	0.41
1:A:413:GLU:O	1:A:413:GLU:HG3	2.21	0.41
1:A:412:PRO:O	1:A:414:TRP:HD1	2.03	0.41
1:A:92:LEU:HA	1:A:92:LEU:HD13	1.87	0.41
2:B:266:TRP:CH2	2:B:423:VAL:HG13	2.55	0.41
1:A:15:GLY:O	1:A:16:MET:HG3	2.22	0.40
2:B:157:PRO:HB3	2:B:184:MET:O	2.21	0.40
2:B:206:ARG:O	2:B:209:LEU:HB2	2.21	0.40
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.21	0.40
1:A:139:THR:HA	1:A:140:PRO:HD2	1.90	0.40
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.03	0.40
1:A:230:MET:SD	1:A:230:MET:N	2.94	0.40
1:A:265:ASN:O	1:A:268:SER:HB2	2.21	0.40
1:A:319:TYR:O	1:A:321:PRO:HD3	2.20	0.40
1:A:360:ALA:HA	1:A:514:GLU:CB	2.51	0.40
1:A:122:GLU:H	1:A:122:GLU:CD	2.25	0.40
1:A:171:PHE:O	1:A:175:ASN:ND2	2.55	0.40
1:A:235:HIS:HB3	1:A:236:PRO:HD2	2.03	0.40
1:A:264:LEU:HD12	1:A:274:ILE:CG2	2.50	0.40
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.51	0.40
1:A:50:ILE:HG13	1:A:143:ARG:HB3	2.03	0.40
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.44	0.40
1:A:342:TYR:HB2	1:A:347:LYS:O	2.22	0.40
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.55	0.40
1:A:31:ILE:O	1:A:35:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	540/560 (96%)	464 (86%)	64 (12%)	12 (2%)	6	7
2	B	396/440 (90%)	343 (87%)	46 (12%)	7 (2%)	8	10
All	All	936/1000 (94%)	807 (86%)	110 (12%)	19 (2%)	7	8

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	122	GLU
1	A	230	MET
2	B	361	HIS
2	B	358	ARG
1	A	91	GLN
1	A	121	ASP
1	A	219	LYS
2	B	67	ASP
2	B	210	LEU
1	A	140	PRO
1	A	361	HIS
1	A	448	ARG
2	B	98	ALA
2	B	195	ILE
1	A	288	ALA
1	A	52	PRO
2	B	241	VAL
1	A	195	ILE

### 5.3.2 Protein sidechains ⓘ

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	485/499 (97%)	434 (90%)	51 (10%)	7	7
2	B	367/400 (92%)	331 (90%)	36 (10%)	8	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	852/899 (95%)	765 (90%)	87 (10%)	<b>7</b> <b>8</b>

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	PRO
1	A	5	ILE
1	A	14	PRO
1	A	24	TRP
1	A	43	LYS
1	A	49	LYS
1	A	64	LYS
1	A	66	LYS
1	A	72	ARG
1	A	109	LEU
1	A	161	GLN
1	A	166	LYS
1	A	175	ASN
1	A	182	GLN
1	A	202	ILE
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	219	LYS
1	A	230	MET
1	A	232	TYR
1	A	234	LEU
1	A	250	ASP
1	A	255	ASN
1	A	270	ILE
1	A	283	LEU
1	A	286	THR
1	A	308	GLU
1	A	311	LYS
1	A	312	GLU
1	A	324	ASP
1	A	325	LEU
1	A	336	GLN
1	A	340	GLN
1	A	357	MET
1	A	358	ARG

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Mol	Chain	Res	Type
1	A	362	THR
1	A	374	LYS
1	A	400	THR
1	A	402	TRP
1	A	403	THR
1	A	410	TRP
1	A	424	LYS
1	A	470	THR
1	A	474	ASN
1	A	493	VAL
1	A	501	TYR
1	A	514	GLU
1	A	517	LEU
1	A	533	LEU
2	B	7	THR
2	B	24	TRP
2	B	61	PHE
2	B	69	THR
2	B	102	LYS
2	B	103	LYS
2	B	104	LYS
2	B	105	SER
2	B	109	LEU
2	B	116	PHE
2	B	167	ILE
2	B	173	LYS
2	B	174	GLN
2	B	179	VAL
2	B	180	ILE
2	B	187	LEU
2	B	192	ASP
2	B	194	GLU
2	B	202	ILE
2	B	203	GLU
2	B	232	TYR
2	B	238	LYS
2	B	276	VAL
2	B	283	LEU
2	B	289	LEU
2	B	300	GLU
2	B	303	LEU
2	B	334	GLN

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Mol	Chain	Res	Type
2	B	336	GLN
2	B	358	ARG
2	B	361	HIS
2	B	368	LEU
2	B	374	LYS
2	B	376	THR
2	B	397	THR
2	B	428	GLN

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	96	HIS
1	A	174	GLN
1	A	255	ASN
1	A	332	GLN
1	A	474	ASN
1	A	500	GLN
2	B	57	ASN
2	B	147	ASN
2	B	182	GLN
2	B	207	GLN
2	B	208	HIS
2	B	242	GLN
2	B	255	ASN
2	B	278	GLN
2	B	334	GLN
2	B	336	GLN
2	B	361	HIS

### 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	0.81	0	1,8,10	5.02	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(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	5.02	115.08	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	TNK	A	999	-	23,29,29	1.25	3 (13%)	24,39,39	3.07	2 (8%)

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	TNK	A	999	-	-	2/12/14/14	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	TNK	C7-C12	-3.95	1.35	1.39
3	A	999	TNK	C11-C12	3.15	1.48	1.41
3	A	999	TNK	C11-N10	2.43	1.37	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	TNK	C11-N10-C9	12.59	125.78	115.14
3	A	999	TNK	C12-C11-N10	-7.75	114.22	126.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	TNK	N8-C17-O17-C18
3	A	999	TNK	C19-C18-O17-C17

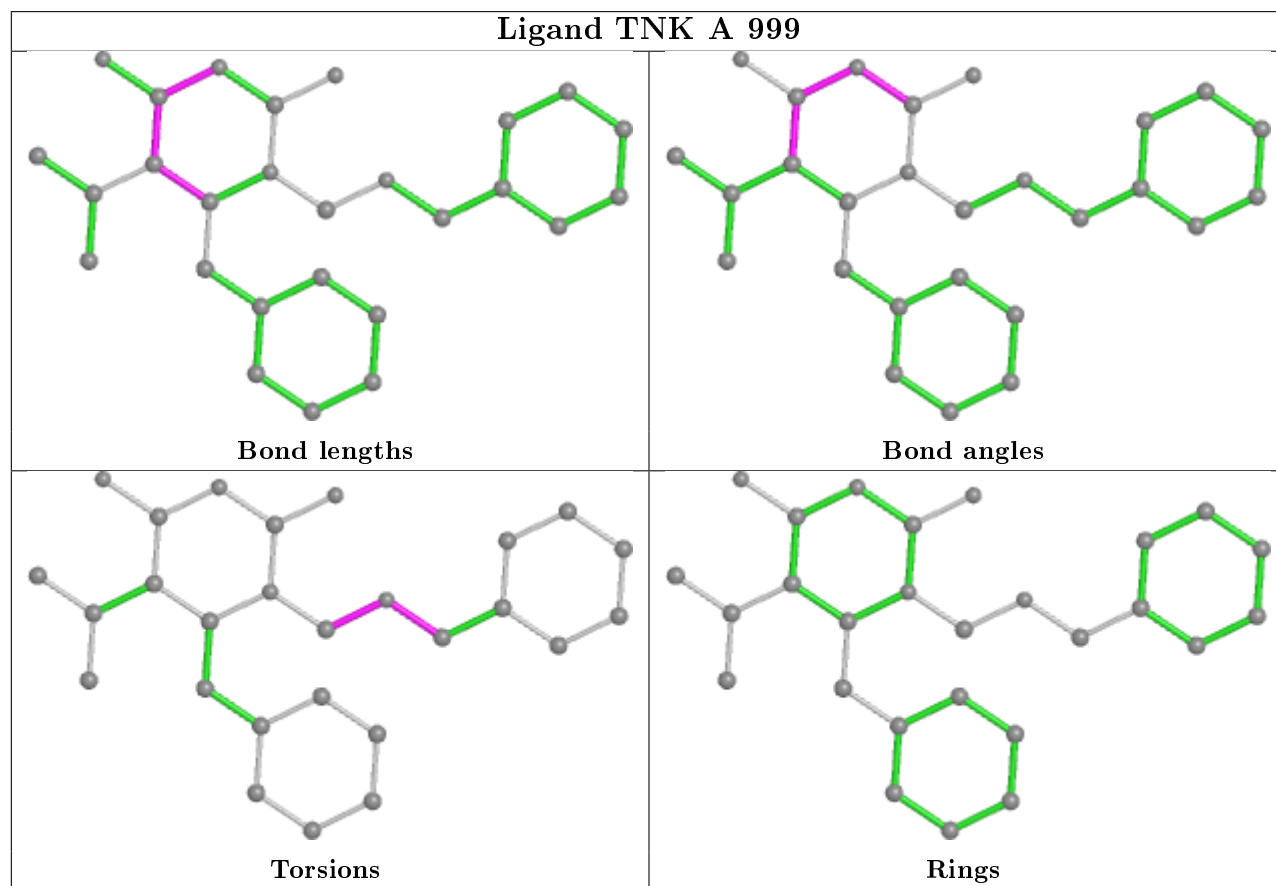


There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	TNK	2	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 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.