



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:34 AM GMT

PDB ID : 1S1V  
Title : Crystal structure of L100I mutant HIV-1 reverse transcriptase in complex with TNK-651  
Authors : Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Stammers, D.K.  
Deposited on : 2004-01-07  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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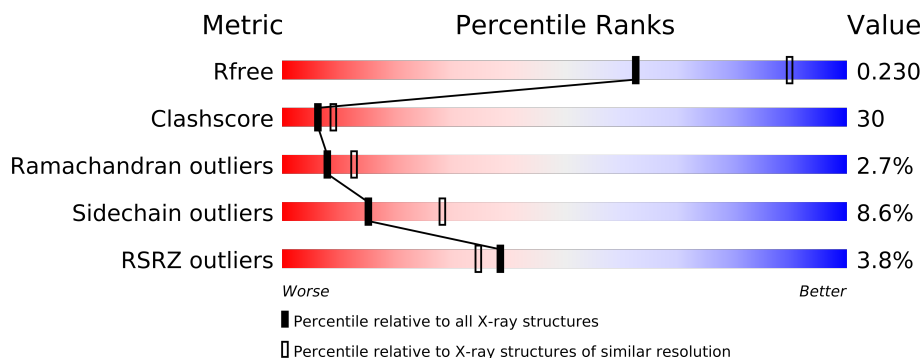
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7803 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4370	2830	727	805	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ILE	LEU	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

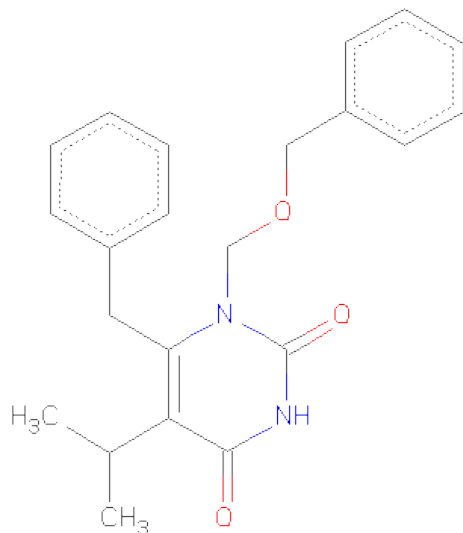
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3339	2172	555	605	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ILE	LEU	ENGINEERED	UNP P04585

- Molecule 3 is 6-BENZYL-1-BENZYLOXYMETHYL-5-ISOPROPYLURACIL (three-letter code: TNK) (formula: C<sub>22</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>).

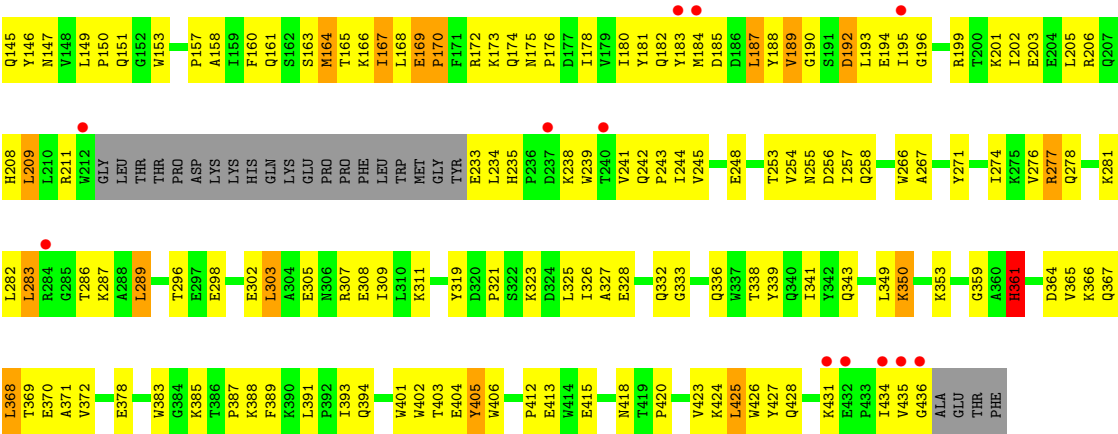


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	2	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	28	Total	O	0	0
			28	28		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.10Å 110.30Å 72.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 2.60 29.51 – 2.59	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.51-2.60) 93.4 (29.51-2.59)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.57Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.233 , 0.313 0.219 , 0.230	Depositor DCC
$R_{free}$ test set	1620 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.1	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 32815 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7803	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.44	0/4477	0.69	2/6085 (0.0%)
2	B	0.46	0/3432	0.69	0/4661
All	All	0.45	0/7909	0.69	2/10746 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	ASN	N-CA-C	-5.32	96.64	111.00
1	A	388	LYS	N-CA-C	-5.07	97.32	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4370	0	4413	272	1
2	B	3339	0	3367	209	0
3	A	27	0	24	5	0
4	A	39	0	0	3	1
4	B	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7803	0	7804	470	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (470) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.59	1.01
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.44	0.98
1:A:182:GLN:HE21	1:A:182:GLN:C	1.68	0.97
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.44	0.96
1:A:270:ILE:HG22	1:A:314:VAL:HG21	1.48	0.96
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.54	0.90
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.53	0.90
1:A:502:ALA:HA	1:A:505:ILE:HD12	1.55	0.88
2:B:235:HIS:O	2:B:238:LYS:HG2	1.73	0.88
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.13	0.87
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.53	0.87
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.57	0.86
2:B:332:GLN:NE2	2:B:424:LYS:HE2	1.89	0.86
2:B:241:VAL:HG22	2:B:350:LYS:HA	1.57	0.85
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.44	0.83
1:A:108:VAL:HG11	1:A:223:LYS:HD2	1.59	0.83
2:B:366:LYS:O	2:B:370:GLU:HG3	1.79	0.83
1:A:17:ASP:O	1:A:83:ARG:HD3	1.79	0.82
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.61	0.82
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.63	0.81
2:B:31:ILE:O	2:B:35:VAL:HG23	1.81	0.81
1:A:388:LYS:HD2	1:A:413:GLU:OE2	1.81	0.81
2:B:266:TRP:CH2	2:B:423:VAL:HG22	2.18	0.78
2:B:350:LYS:HE2	2:B:378:GLU:OE1	1.82	0.78
1:A:16:MET:HE3	4:A:1004:HOH:O	1.82	0.78
1:A:16:MET:CE	1:A:83:ARG:HG2	2.14	0.78
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.30	0.78
1:A:228:LEU:N	1:A:228:LEU:HD12	1.98	0.78
2:B:332:GLN:HE22	2:B:424:LYS:HE2	1.46	0.78
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.50	0.77
1:A:278:GLN:O	1:A:282:LEU:HD13	1.85	0.77
2:B:195:ILE:HG23	2:B:196:GLY:H	1.49	0.76
1:A:98:ALA:HB2	1:A:349:LEU:O	1.87	0.74
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.17	0.74
2:B:163:SER:O	2:B:167:ILE:HG23	1.86	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:344:GLU:OE1	1:A:347:LYS:HD2	1.86	0.74
1:A:30:LYS:HE2	1:A:71:TRP:CH2	2.23	0.74
1:A:376:THR:O	1:A:380:ILE:HG12	1.88	0.73
1:A:94:ILE:HG21	1:A:230:MET:CE	2.19	0.73
1:A:120:LEU:HD13	1:A:125:ARG:HG2	1.71	0.73
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.18	0.72
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.69	0.72
1:A:116:PHE:CE2	1:A:151:GLN:HG2	2.25	0.72
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.20	0.71
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.26	0.71
1:A:136:ASN:C	1:A:138:GLU:H	1.91	0.70
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.55	0.70
1:A:19:PRO:O	1:A:56:TYR:HA	1.90	0.70
2:B:139:THR:HG22	2:B:140:PRO:O	1.90	0.70
2:B:195:ILE:HG23	2:B:196:GLY:N	2.07	0.69
1:A:516:GLU:O	1:A:520:GLN:HG3	1.92	0.69
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.75	0.69
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.28	0.69
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.28	0.69
1:A:362:THR:HG22	1:A:363:ASN:H	1.58	0.68
1:A:225:PRO:HA	1:A:226:PRO:C	2.12	0.68
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.76	0.68
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.07	0.68
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.06	0.68
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.29	0.67
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.75	0.67
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.77	0.67
1:A:317:VAL:HG12	1:A:318:TYR:N	2.11	0.66
2:B:323:LYS:NZ	2:B:323:LYS:HB2	2.10	0.66
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.76	0.66
1:A:420:PRO:HA	1:A:421:PRO:C	2.14	0.66
1:A:136:ASN:HB2	1:A:138:GLU:HG3	1.77	0.66
2:B:35:VAL:O	2:B:39:THR:HG23	1.96	0.66
2:B:208:HIS:O	2:B:211:ARG:HG2	1.95	0.66
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.11	0.65
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.60	0.65
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.31	0.65
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.77	0.65
1:A:40:GLU:HA	1:A:43:LYS:HE2	1.79	0.65
1:A:312:GLU:N	1:A:313:PRO:HD3	2.12	0.65
1:A:63:ILE:HA	1:A:71:TRP:HZ3	1.62	0.65
2:B:78:ARG:O	2:B:82:LYS:HG3	1.96	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.32	0.64
1:A:11:LYS:O	1:A:85:GLN:HB3	1.97	0.64
2:B:61:PHE:HE1	2:B:74:LEU:HD23	1.63	0.64
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.78	0.64
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.64
1:A:323:LYS:NZ	1:A:344:GLU:HG2	2.13	0.64
1:A:271:TYR:OH	1:A:313:PRO:HA	1.98	0.64
2:B:365:VAL:O	2:B:369:THR:HG23	1.98	0.64
1:A:451:LYS:HD3	1:A:471:ASP:OD2	1.98	0.63
2:B:424:LYS:C	2:B:424:LYS:HD3	2.18	0.63
2:B:195:ILE:HG12	2:B:199:ARG:HH21	1.62	0.63
1:A:475:GLN:HG3	1:A:476:LYS:N	2.12	0.63
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.33	0.63
1:A:255:ASN:O	1:A:259:LYS:HG2	1.99	0.62
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.46	0.62
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.80	0.62
1:A:79:GLU:HB3	1:A:83:ARG:NH1	2.14	0.62
1:A:257:ILE:O	1:A:261:VAL:HG23	2.00	0.62
1:A:2:ILE:HG22	1:A:3:SER:N	2.14	0.62
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.81	0.62
2:B:73:LYS:NZ	2:B:73:LYS:HB3	2.14	0.61
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.14	0.61
1:A:503:LEU:HD13	1:A:535:TRP:CG	2.36	0.61
2:B:278:GLN:NE2	2:B:281:LYS:HD2	2.15	0.60
1:A:28:GLU:O	1:A:32:LYS:HG3	2.01	0.60
2:B:319:TYR:HE1	2:B:321:PRO:HG3	1.66	0.60
1:A:368:LEU:O	1:A:372:VAL:HG23	2.01	0.60
2:B:368:LEU:O	2:B:372:VAL:HG23	2.01	0.60
2:B:308:GLU:O	2:B:311:LYS:HB2	2.01	0.60
2:B:434:ILE:HG22	2:B:435:VAL:HG13	1.82	0.60
1:A:536:VAL:HG12	2:B:258:GLN:HB3	1.83	0.60
2:B:254:VAL:O	2:B:258:GLN:HG3	2.00	0.60
2:B:79:GLU:O	2:B:83:ARG:HG3	2.01	0.60
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.12	0.60
1:A:40:GLU:HA	1:A:43:LYS:CE	2.32	0.60
2:B:424:LYS:HZ3	2:B:425:LEU:HD12	1.66	0.59
1:A:228:LEU:CD1	1:A:228:LEU:N	2.64	0.59
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.14	0.59
1:A:312:GLU:N	1:A:313:PRO:CD	2.64	0.59
1:A:260:LEU:HG	1:A:264:LEU:CD2	2.33	0.59
1:A:419:THR:HG22	1:A:419:THR:O	2.02	0.59
2:B:423:VAL:O	2:B:427:TYR:HD2	1.83	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:97:PRO:O	2:B:99:GLY:N	2.36	0.59
1:A:371:ALA:O	1:A:375:ILE:HG13	2.03	0.59
2:B:94:ILE:HD11	2:B:182:GLN:H	1.68	0.59
2:B:203:GLU:HA	2:B:206:ARG:HB2	1.85	0.59
1:A:246:LEU:O	1:A:307:ARG:NH1	2.32	0.59
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.32	0.58
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.34	0.58
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.83	0.58
1:A:122:GLU:N	1:A:122:GLU:OE1	2.36	0.58
1:A:2:ILE:HG22	1:A:3:SER:H	1.69	0.58
1:A:116:PHE:HE2	1:A:151:GLN:HG2	1.67	0.58
2:B:88:TRP:CZ3	2:B:93:GLY:N	2.71	0.58
1:A:48:SER:O	1:A:144:TYR:HA	2.03	0.58
2:B:27:THR:O	2:B:31:ILE:HG13	2.03	0.58
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.04	0.58
1:A:33:ALA:O	1:A:36:GLU:HB3	2.04	0.57
2:B:98:ALA:HA	2:B:101:LYS:NZ	2.19	0.57
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.38	0.57
1:A:522:ILE:O	1:A:526:ILE:HG13	2.04	0.57
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.40	0.57
2:B:169:GLU:HG2	2:B:173:LYS:HZ3	1.70	0.57
1:A:323:LYS:HZ3	1:A:344:GLU:HG2	1.69	0.57
2:B:97:PRO:C	2:B:99:GLY:H	2.07	0.57
1:A:380:ILE:O	1:A:384:GLY:HA2	2.05	0.57
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.19	0.56
1:A:16:MET:HE1	1:A:83:ARG:HG2	1.84	0.56
2:B:160:PHE:CD1	2:B:160:PHE:O	2.57	0.56
1:A:162:SER:O	1:A:165:THR:HB	2.06	0.56
1:A:114:ALA:O	1:A:117:SER:HB2	2.05	0.56
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.40	0.56
2:B:164:MET:O	2:B:168:LEU:HG	2.05	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.40	0.56
2:B:241:VAL:CG2	2:B:350:LYS:HA	2.33	0.56
2:B:173:LYS:O	2:B:176:PRO:HD3	2.06	0.56
1:A:188:TYR:CD2	3:A:999:TNK:H2	2.41	0.56
1:A:90:VAL:O	1:A:91:GLN:C	2.44	0.55
1:A:492:GLU:HA	1:A:530:LYS:O	2.06	0.55
2:B:202:ILE:O	2:B:205:LEU:N	2.38	0.55
1:A:254:VAL:HB	1:A:289:LEU:HA	1.87	0.55
1:A:202:ILE:HG22	1:A:203:GLU:N	2.22	0.55
1:A:289:LEU:HD22	1:A:289:LEU:H	1.70	0.55
1:A:110:ASP:O	1:A:217:PRO:HD2	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:50:ILE:CG1	2:B:143:ARG:HB3	2.37	0.55
2:B:205:LEU:HD13	2:B:209:LEU:HD22	1.88	0.55
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.06	0.55
2:B:107:THR:O	2:B:189:VAL:HG23	2.06	0.55
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.37	0.55
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.42	0.55
1:A:11:LYS:NZ	4:A:1003:HOH:O	2.39	0.55
2:B:13:LYS:HE2	2:B:86:ASP:OD2	2.07	0.55
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.88	0.55
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.55
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.42	0.54
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.70	0.54
2:B:178:ILE:HG23	2:B:190:GLY:O	2.07	0.54
1:A:136:ASN:C	1:A:138:GLU:N	2.61	0.54
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.89	0.54
2:B:98:ALA:HA	2:B:101:LYS:HZ1	1.73	0.54
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.90	0.54
2:B:423:VAL:O	2:B:427:TYR:CD2	2.61	0.54
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.36	0.54
1:A:108:VAL:CG1	1:A:223:LYS:HD2	2.33	0.53
2:B:323:LYS:HB2	2:B:323:LYS:HZ2	1.72	0.53
1:A:182:GLN:NE2	1:A:182:GLN:C	2.51	0.53
2:B:97:PRO:O	2:B:100:ILE:HG22	2.09	0.53
1:A:293:ILE:N	1:A:293:ILE:HD12	2.22	0.53
1:A:94:ILE:HG21	1:A:230:MET:HE1	1.88	0.53
1:A:418:ASN:C	1:A:420:PRO:HD3	2.29	0.53
2:B:328:GLU:O	2:B:339:TYR:HA	2.08	0.53
2:B:57:ASN:HD21	2:B:131:THR:CB	2.22	0.53
2:B:111:VAL:HG22	2:B:185:ASP:O	2.08	0.53
1:A:486:LEU:O	1:A:528:LYS:NZ	2.42	0.53
1:A:248:GLU:O	1:A:249:LYS:HG3	2.08	0.53
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.89	0.53
2:B:94:ILE:HD11	2:B:181:TYR:HD2	1.74	0.53
1:A:112:GLY:O	1:A:114:ALA:N	2.38	0.53
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.43	0.53
1:A:169:GLU:O	1:A:173:LYS:HG3	2.09	0.53
1:A:27:THR:O	1:A:31:ILE:HG13	2.09	0.53
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.90	0.53
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.44	0.53
2:B:46:LYS:HE2	2:B:116:PHE:HD2	1.74	0.53
1:A:331:LYS:CE	1:A:334:GLN:HA	2.38	0.52
1:A:476:LYS:O	1:A:480:GLN:HB2	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:420:PRO:HB2	2:B:423:VAL:CG2	2.33	0.52
2:B:88:TRP:CE3	2:B:88:TRP:HA	2.44	0.52
2:B:305:GLU:O	2:B:309:ILE:HG13	2.10	0.52
1:A:252:TRP:NE1	1:A:295:LEU:HD11	2.25	0.52
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.75	0.52
1:A:502:ALA:HA	1:A:505:ILE:CD1	2.33	0.52
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.44	0.52
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.10	0.52
1:A:171:PHE:O	1:A:175:ASN:ND2	2.43	0.52
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.92	0.52
2:B:10:VAL:HG11	2:B:153:TRP:CZ2	2.44	0.52
1:A:289:LEU:N	1:A:289:LEU:HD22	2.25	0.52
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.43	0.52
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.40	0.52
1:A:474:ASN:O	1:A:478:GLU:HG3	2.09	0.52
1:A:514:GLU:HG3	1:A:515:SER:N	2.26	0.51
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.45	0.51
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.91	0.51
2:B:195:ILE:HG12	2:B:199:ARG:NH2	2.24	0.51
2:B:97:PRO:C	2:B:99:GLY:N	2.64	0.51
1:A:182:GLN:HE21	1:A:183:TYR:N	2.08	0.51
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.46	0.51
1:A:122:GLU:CD	1:A:122:GLU:H	2.15	0.51
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.92	0.51
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.45	0.51
2:B:401:TRP:O	2:B:404:GLU:N	2.37	0.51
2:B:248:GLU:HG2	2:B:307:ARG:CZ	2.40	0.51
2:B:205:LEU:O	2:B:208:HIS:HB3	2.12	0.50
1:A:317:VAL:CG1	1:A:318:TYR:N	2.75	0.50
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.46	0.50
1:A:49:LYS:HA	1:A:143:ARG:O	2.11	0.50
1:A:253:THR:HB	1:A:290:THR:O	2.11	0.50
2:B:11:LYS:N	2:B:85:GLN:OE1	2.41	0.50
2:B:169:GLU:O	2:B:172:ARG:N	2.44	0.50
1:A:363:ASN:O	1:A:366:LYS:HB3	2.10	0.50
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.92	0.50
2:B:205:LEU:CD1	2:B:209:LEU:HD22	2.42	0.50
2:B:413:GLU:OE2	2:B:413:GLU:HA	2.11	0.50
2:B:88:TRP:HE3	2:B:88:TRP:HA	1.75	0.50
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.47	0.50
2:B:125:ARG:NE	2:B:147:ASN:HA	2.27	0.50
2:B:195:ILE:CG2	2:B:196:GLY:H	2.21	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.94	0.49
1:A:122:GLU:HA	1:A:125:ARG:NE	2.27	0.49
1:A:168:LEU:O	1:A:172:ARG:HG3	2.11	0.49
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.11	0.49
1:A:89:GLU:HG3	1:A:89:GLU:O	2.12	0.49
2:B:349:LEU:O	2:B:350:LYS:HB2	2.12	0.49
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.93	0.49
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.75	0.49
1:A:63:ILE:CA	1:A:71:TRP:HZ3	2.24	0.49
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.47	0.49
2:B:169:GLU:O	2:B:173:LYS:HD3	2.13	0.49
2:B:195:ILE:CD1	2:B:199:ARG:NE	2.75	0.49
1:A:112:GLY:C	1:A:114:ALA:H	2.16	0.49
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.42	0.49
1:A:155:GLY:O	1:A:159:ILE:HG13	2.13	0.49
1:A:235:HIS:HB2	1:A:238:LYS:O	2.13	0.49
1:A:79:GLU:O	1:A:82:LYS:HG2	2.12	0.49
1:A:95:PRO:HG3	2:B:136:ASN:O	2.13	0.48
2:B:6:GLU:HA	2:B:6:GLU:OE1	2.12	0.48
1:A:448:ARG:NE	1:A:474:ASN:HB2	2.28	0.48
2:B:104:LYS:NZ	2:B:192:ASP:HB3	2.28	0.48
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.95	0.48
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.43	0.48
1:A:317:VAL:CG2	1:A:347:LYS:HB3	2.38	0.48
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.96	0.48
2:B:43:LYS:C	2:B:45:GLY:H	2.17	0.48
2:B:109:LEU:HD11	2:B:205:LEU:HD12	1.95	0.48
1:A:283:LEU:HD12	1:A:283:LEU:N	2.28	0.48
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.14	0.48
2:B:10:VAL:HG11	2:B:153:TRP:HZ2	1.79	0.48
1:A:340:GLN:CB	1:A:351:THR:HG22	2.44	0.48
1:A:181:TYR:HB2	3:A:999:TNK:H161	1.96	0.48
1:A:332:GLN:HG2	1:A:332:GLN:O	2.14	0.48
1:A:181:TYR:HH	1:A:183:TYR:HD2	1.60	0.48
2:B:169:GLU:CG	2:B:173:LYS:HZ3	2.27	0.48
2:B:325:LEU:HA	2:B:343:GLN:HG2	1.96	0.47
1:A:26:LEU:O	1:A:31:ILE:HD11	2.13	0.47
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.48	0.47
1:A:360:ALA:O	1:A:361:HIS:HB3	2.14	0.47
2:B:242:GLN:OE1	2:B:242:GLN:HA	2.13	0.47
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.96	0.47
1:A:289:LEU:H	1:A:289:LEU:CD2	2.26	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:333:GLY:O	2:B:336:GLN:HB2	2.14	0.47
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.96	0.47
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.95	0.47
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.78	0.47
1:A:57:ASN:HA	1:A:129:ALA:O	2.15	0.47
2:B:94:ILE:HD11	2:B:181:TYR:CD2	2.49	0.47
2:B:125:ARG:HG2	2:B:146:TYR:O	2.15	0.47
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.44	0.47
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.45	0.47
2:B:136:ASN:O	2:B:137:ASN:HB2	2.15	0.47
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.49	0.47
2:B:368:LEU:O	2:B:371:ALA:HB3	2.14	0.47
1:A:460:ASN:HA	2:B:286:THR:O	2.14	0.47
2:B:332:GLN:HE22	2:B:428:GLN:HB2	1.79	0.47
2:B:241:VAL:O	2:B:241:VAL:HG12	2.15	0.47
1:A:79:GLU:HA	1:A:82:LYS:HG2	1.96	0.47
2:B:276:VAL:HA	2:B:302:GLU:OE2	2.14	0.46
1:A:186:ASP:CG	1:A:223:LYS:HE3	2.35	0.46
1:A:58:THR:HG23	1:A:76:ASP:O	2.15	0.46
1:A:447:ASN:O	1:A:451:LYS:N	2.48	0.46
1:A:402:TRP:CD1	1:A:402:TRP:C	2.89	0.46
1:A:50:ILE:HG21	1:A:145:GLN:HG2	1.98	0.46
2:B:169:GLU:HA	2:B:173:LYS:HZ2	1.79	0.46
1:A:77:PHE:O	1:A:78:ARG:C	2.54	0.46
1:A:409:THR:O	1:A:410:TRP:HB2	2.14	0.46
2:B:173:LYS:N	2:B:173:LYS:HD2	2.30	0.46
1:A:8:VAL:O	1:A:121:ASP:HB2	2.15	0.46
1:A:312:GLU:H	1:A:313:PRO:HD3	1.81	0.46
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.29	0.46
1:A:3:SER:HB3	1:A:5:ILE:CG1	2.37	0.46
2:B:116:PHE:HE1	2:B:151:GLN:CG	2.28	0.46
1:A:356:ARG:NH1	1:A:356:ARG:CG	2.78	0.46
1:A:169:GLU:HB2	1:A:170:PRO:HD3	1.97	0.46
1:A:118:VAL:O	1:A:148:VAL:HB	2.16	0.46
1:A:362:THR:HG22	1:A:363:ASN:N	2.28	0.46
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.97	0.46
1:A:415:GLU:HG2	1:A:416:PHE:O	2.16	0.46
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.46	0.45
2:B:131:THR:HG1	2:B:143:ARG:HH11	1.64	0.45
1:A:317:VAL:HG12	1:A:318:TYR:O	2.17	0.45
2:B:195:ILE:CG1	2:B:199:ARG:NE	2.78	0.45
1:A:345:PRO:O	1:A:346:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:245:VAL:HG23	2:B:245:VAL:O	2.16	0.45
2:B:326:ILE:HG22	2:B:327:ALA:N	2.31	0.45
1:A:468:THR:O	1:A:469:LEU:HD23	2.16	0.45
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.16	0.45
2:B:158:ALA:O	2:B:161:GLN:HB2	2.16	0.45
1:A:257:ILE:HG22	1:A:283:LEU:HD11	1.97	0.45
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.97	0.45
1:A:434:ILE:CG2	1:A:437:ALA:HB2	2.46	0.45
1:A:208:HIS:O	1:A:211:ARG:HB3	2.16	0.45
2:B:39:THR:O	2:B:42:GLU:HB3	2.17	0.45
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.37	0.45
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.99	0.45
1:A:58:THR:CG2	1:A:76:ASP:O	2.65	0.45
1:A:266:TRP:C	1:A:266:TRP:CD1	2.90	0.45
2:B:139:THR:HG23	2:B:140:PRO:CD	2.47	0.45
1:A:118:VAL:HB	1:A:149:LEU:HD13	1.99	0.45
1:A:100:ILE:HD12	2:B:136:ASN:HD21	1.82	0.44
1:A:516:GLU:O	1:A:519:ASN:HB2	2.18	0.44
1:A:418:ASN:O	1:A:420:PRO:HD3	2.17	0.44
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.87	0.44
1:A:317:VAL:HG12	1:A:318:TYR:H	1.78	0.44
1:A:120:LEU:O	1:A:122:GLU:N	2.50	0.44
1:A:498:ASP:HA	1:A:536:VAL:O	2.17	0.44
2:B:118:VAL:HG12	2:B:119:PRO:O	2.18	0.44
1:A:181:TYR:CZ	1:A:183:TYR:HB2	2.52	0.44
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.52	0.44
2:B:116:PHE:HE1	2:B:151:GLN:CD	2.20	0.44
1:A:340:GLN:HA	1:A:351:THR:HA	1.99	0.44
2:B:332:GLN:HE22	2:B:424:LYS:CE	2.24	0.44
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.86	0.44
1:A:169:GLU:N	1:A:170:PRO:CD	2.79	0.44
2:B:53:GLU:CD	2:B:53:GLU:H	2.21	0.44
2:B:63:ILE:HG13	2:B:72:ARG:HB3	1.97	0.44
2:B:105:SER:HA	2:B:234:LEU:O	2.17	0.44
2:B:303:LEU:HD13	2:B:307:ARG:NH2	2.33	0.44
1:A:508:ALA:O	1:A:509:GLN:C	2.56	0.44
2:B:163:SER:O	2:B:167:ILE:CG2	2.62	0.44
1:A:115:TYR:CG	1:A:151:GLN:NE2	2.86	0.44
2:B:73:LYS:HZ2	2:B:73:LYS:HB3	1.82	0.44
1:A:399:GLU:O	1:A:403:THR:HB	2.17	0.44
1:A:63:ILE:O	1:A:63:ILE:HD12	2.18	0.44
2:B:435:VAL:HG23	2:B:436:GLY:N	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:457:TYR:C	1:A:457:TYR:CD1	2.91	0.44
1:A:100:ILE:HG12	3:A:999:TNK:H6	1.99	0.44
1:A:279:LEU:CD2	1:A:302:GLU:OE1	2.66	0.44
2:B:46:LYS:CE	2:B:116:PHE:HD2	2.31	0.43
2:B:388:LYS:HE2	2:B:415:GLU:HB3	2.00	0.43
1:A:161:GLN:OE1	1:A:161:GLN:HA	2.18	0.43
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.53	0.43
1:A:434:ILE:HB	1:A:437:ALA:HB3	2.01	0.43
2:B:173:LYS:C	2:B:175:ASN:N	2.72	0.43
1:A:228:LEU:H	1:A:228:LEU:HD12	1.81	0.43
1:A:479:LEU:O	1:A:521:ILE:HD11	2.18	0.43
2:B:353:LYS:HB2	2:B:353:LYS:HE3	1.84	0.43
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.84	0.43
2:B:277:ARG:HG2	2:B:278:GLN:H	1.84	0.43
2:B:393:ILE:HG12	2:B:394:GLN:N	2.34	0.43
1:A:377:THR:O	1:A:381:VAL:HG23	2.18	0.43
2:B:170:PRO:O	2:B:174:GLN:HG3	2.18	0.43
1:A:132:ILE:HA	1:A:133:PRO:HD3	1.84	0.43
2:B:245:VAL:HG13	2:B:431:LYS:HB2	2.01	0.43
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.64	0.43
2:B:108:VAL:HA	2:B:187:LEU:O	2.18	0.43
1:A:232:TYR:HA	1:A:240:THR:O	2.19	0.43
2:B:404:GLU:HB2	2:B:405:TYR:CE1	2.54	0.43
1:A:228:LEU:CD1	1:A:228:LEU:H	2.31	0.43
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.54	0.43
1:A:229:TRP:O	1:A:232:TYR:HB2	2.18	0.42
1:A:439:THR:HA	1:A:494:ASN:HB2	2.01	0.42
1:A:254:VAL:HB	1:A:289:LEU:O	2.18	0.42
1:A:400:THR:O	1:A:403:THR:HG22	2.19	0.42
1:A:465:LYS:HG2	1:A:466:VAL:N	2.33	0.42
1:A:182:GLN:NE2	1:A:183:TYR:N	2.67	0.42
2:B:169:GLU:O	2:B:172:ARG:HB2	2.19	0.42
1:A:317:VAL:CG1	1:A:318:TYR:H	2.33	0.42
2:B:8:VAL:HG23	2:B:9:PRO:HD2	2.01	0.42
2:B:406:TRP:CH2	2:B:412:PRO:HD2	2.55	0.42
1:A:84:THR:HB	1:A:154:LYS:HD3	2.01	0.42
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.54	0.42
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.74	0.42
1:A:54:ASN:O	1:A:56:TYR:N	2.52	0.42
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.35	0.42
1:A:170:PRO:O	1:A:174:GLN:HG3	2.20	0.42
2:B:253:THR:O	2:B:256:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:442:VAL:HG22	1:A:496:VAL:O	2.19	0.42
1:A:24:TRP:CB	1:A:61:PHE:HE1	2.32	0.42
1:A:236:PRO:HB3	3:A:999:TNK:C22	2.50	0.42
2:B:326:ILE:O	2:B:341:ILE:HA	2.20	0.42
1:A:94:ILE:CG2	1:A:230:MET:HE2	2.48	0.42
1:A:451:LYS:O	1:A:471:ASP:N	2.53	0.42
2:B:278:GLN:HG3	2:B:298:GLU:HB3	2.02	0.42
2:B:254:VAL:O	2:B:255:ASN:C	2.58	0.42
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.85	0.42
1:A:438:GLU:OE1	1:A:459:THR:CB	2.68	0.42
1:A:379:SER:O	1:A:380:ILE:C	2.57	0.42
2:B:139:THR:CG2	2:B:140:PRO:N	2.83	0.42
1:A:489:SER:HB2	1:A:493:VAL:HG13	2.02	0.42
2:B:401:TRP:O	2:B:402:TRP:C	2.57	0.42
1:A:339:TYR:CD1	1:A:339:TYR:C	2.93	0.42
3:A:999:TNK:H131	3:A:999:TNK:H172	1.80	0.42
1:A:270:ILE:CG2	1:A:314:VAL:CG2	2.93	0.42
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.53	0.42
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.50	0.42
1:A:79:GLU:HA	1:A:82:LYS:CD	2.49	0.41
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.83	0.41
1:A:28:GLU:HG3	1:A:29:GLU:N	2.35	0.41
2:B:88:TRP:CH2	2:B:93:GLY:N	2.88	0.41
2:B:389:PHE:HB3	2:B:391:LEU:HD21	2.02	0.41
1:A:9:PRO:HG2	2:B:53:GLU:HG3	2.02	0.41
1:A:94:ILE:HG22	1:A:229:TRP:CH2	2.55	0.41
1:A:393:ILE:HB	1:A:423:VAL:HG22	2.00	0.41
1:A:82:LYS:HA	4:A:1007:HOH:O	2.19	0.41
1:A:70:LYS:HE2	1:A:70:LYS:HB3	1.88	0.41
2:B:168:LEU:O	2:B:169:GLU:C	2.58	0.41
1:A:254:VAL:HG23	1:A:293:ILE:HD11	2.01	0.41
1:A:496:VAL:HA	1:A:534:ALA:O	2.20	0.41
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.20	0.41
2:B:125:ARG:O	2:B:126:LYS:C	2.59	0.41
2:B:41:MET:HE2	2:B:41:MET:HB3	1.91	0.41
1:A:95:PRO:HD2	1:A:229:TRP:HH2	1.85	0.41
1:A:279:LEU:HD23	1:A:302:GLU:OE1	2.21	0.41
1:A:536:VAL:CG1	2:B:258:GLN:HB3	2.49	0.41
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.56	0.41
1:A:120:LEU:CD2	1:A:121:ASP:N	2.83	0.41
1:A:138:GLU:HB3	1:A:139:THR:H	1.51	0.41
1:A:503:LEU:HD13	1:A:535:TRP:CB	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:337:TRP:CZ3	1:A:368:LEU:HD23	2.55	0.41
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.21	0.41
2:B:364:ASP:O	2:B:367:GLN:N	2.54	0.41
1:A:95:PRO:HB3	2:B:136:ASN:ND2	2.37	0.40
1:A:132:ILE:O	1:A:141:GLY:HA3	2.21	0.40
1:A:253:THR:HA	1:A:291:GLU:O	2.22	0.40
1:A:15:GLY:O	1:A:16:MET:C	2.60	0.40
1:A:114:ALA:HA	1:A:117:SER:HB2	2.02	0.40
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.57	0.40
1:A:103:LYS:HB3	1:A:191:SER:O	2.21	0.40
1:A:401:TRP:HB2	1:A:425:LEU:HD21	2.03	0.40
1:A:96:HIS:CD2	1:A:98:ALA:H	2.40	0.40
1:A:486:LEU:HB3	1:A:524:GLN:HB3	2.03	0.40
2:B:151:GLN:HG3	2:B:151:GLN:H	1.55	0.40
2:B:46:LYS:HG2	2:B:116:PHE:CD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:GLU:OE1	4:A:1057:HOH:O[1_556]	2.15	0.05

## 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	527/560 (94%)	460 (87%)	49 (9%)	18 (3%)	6	8
2	B	396/440 (90%)	344 (87%)	45 (11%)	7 (2%)	13	25
All	All	923/1000 (92%)	804 (87%)	94 (10%)	25 (3%)	8	13

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	272	PRO
1	A	16	MET
1	A	85	GLN
1	A	112	GLY
1	A	296	THR
1	A	313	PRO
2	B	98	ALA
2	B	361	HIS
1	A	95	PRO
1	A	113	ASP
1	A	361	HIS
1	A	420	PRO
2	B	193	LEU
1	A	78	ARG
1	A	121	ASP
2	B	40	GLU
2	B	166	LYS
2	B	350	LYS
1	A	91	GLN
1	A	52	PRO
1	A	312	GLU
2	B	169	GLU
1	A	55	PRO

### 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	478/499 (96%)	431 (90%)	47 (10%)	12	21
2	B	367/400 (92%)	341 (93%)	26 (7%)	21	40
All	All	845/899 (94%)	772 (91%)	73 (9%)	15	28

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU

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Mol	Chain	Res	Type
1	A	53	GLU
1	A	69	THR
1	A	89	GLU
1	A	92	LEU
1	A	102	LYS
1	A	109	LEU
1	A	120	LEU
1	A	122	GLU
1	A	123	ASP
1	A	135	ILE
1	A	166	LYS
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	195	ILE
1	A	205	LEU
1	A	211	ARG
1	A	229	TRP
1	A	230	MET
1	A	237	ASP
1	A	238	LYS
1	A	249	LYS
1	A	255	ASN
1	A	266	TRP
1	A	313	PRO
1	A	325	LEU
1	A	336	GLN
1	A	340	GLN
1	A	361	HIS
1	A	362	THR
1	A	369	THR
1	A	402	TRP
1	A	404	GLU
1	A	420	PRO
1	A	448	ARG
1	A	452	LEU
1	A	468	THR
1	A	474	ASN
1	A	475	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL

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Mol	Chain	Res	Type
1	A	500	GLN
1	A	501	TYR
1	A	517	LEU
1	A	533	LEU
2	B	29	GLU
2	B	46	LYS
2	B	73	LYS
2	B	88	TRP
2	B	113	ASP
2	B	164	MET
2	B	165	THR
2	B	167	ILE
2	B	170	PRO
2	B	187	LEU
2	B	189	VAL
2	B	192	ASP
2	B	194	GLU
2	B	209	LEU
2	B	233	GLU
2	B	243	PRO
2	B	277	ARG
2	B	283	LEU
2	B	287	LYS
2	B	289	LEU
2	B	303	LEU
2	B	361	HIS
2	B	368	LEU
2	B	403	THR
2	B	405	TYR
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	96	HIS
1	A	136	ASN
1	A	151	GLN
1	A	174	GLN
1	A	175	ASN
1	A	182	GLN
1	A	242	GLN

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	474	ASN
1	A	475	GLN
1	A	500	GLN
1	A	507	GLN
1	A	512	GLN
2	B	57	ASN
2	B	161	GLN
2	B	175	ASN
2	B	197	GLN
2	B	208	HIS
2	B	235	HIS
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	361	HIS
2	B	394	GLN
2	B	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	7,7,8	7.12	2 (28%)	6,8,10	5.50	5 (83%)

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	-	1/3/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	O-C	18.53	1.24	1.11
1	A	280	CSD	CA-C	2.62	1.53	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	CA-CB-SG	10.19	125.35	110.82
1	A	280	CSD	C-CA-N	-5.46	108.38	113.83
1	A	280	CSD	OD2-SG-OD1	5.22	118.05	109.39
1	A	280	CSD	OD2-SG-CB	3.45	111.30	97.42
1	A	280	CSD	OD1-SG-CB	3.00	113.21	105.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

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	-	29,29,29	1.54	3 (10%)	34,39,39	1.30	4 (11%)

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	-	-	0/12/14/14	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	C9-N8	3.31	1.42	1.38
3	A	999	TNK	C13-C7	3.25	1.54	1.50
3	A	999	TNK	C7-N8	3.07	1.42	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	TNK	C7-C13-C1	3.60	120.02	114.65
3	A	999	TNK	C7-C12-C14	3.55	126.08	121.72
3	A	999	TNK	C11-C12-C14	-2.64	114.91	122.67
3	A	999	TNK	C17-N8-C9	-2.14	116.44	118.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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	534/560 (95%)	-0.12	17 (3%)	45 42	39, 75, 120, 150	0
2	B	404/440 (91%)	-0.05	19 (4%)	30 27	38, 74, 125, 150	0
All	All	938/1000 (93%)	-0.09	36 (3%)	38 35	38, 74, 122, 150	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	436	GLY	4.9
2	B	435	VAL	4.6
1	A	136	ASN	4.4
1	A	220	LYS	4.0
1	A	53	GLU	4.0
2	B	240	THR	4.0
2	B	69	THR	3.9
1	A	1	PRO	3.8
2	B	104	LYS	3.8
2	B	94	ILE	3.8
2	B	434	ILE	3.7
2	B	212	TRP	3.5
1	A	245	VAL	3.5
2	B	88	TRP	3.5
1	A	221	HIS	3.4
1	A	89	GLU	3.4
2	B	70	LYS	3.2
1	A	446	ALA	2.9
2	B	195	ILE	2.9
1	A	470	THR	2.8
2	B	183	TYR	2.7
2	B	184	MET	2.6
1	A	301	LEU	2.5
2	B	284	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	91	GLN	2.5
1	A	22	LYS	2.4
1	A	52	PRO	2.4
2	B	432	GLU	2.3
1	A	448	ARG	2.3
2	B	431	LYS	2.3
1	A	135	ILE	2.2
2	B	6	GLU	2.2
1	A	69	THR	2.1
2	B	7	THR	2.1
1	A	64	LYS	2.1
2	B	237	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	A	280	8/9	0.12	-0.66	74,75,88,95	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TNK	A	999	27/27	0.16	0.19	42,61,82,86	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.