



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:43 PM GMT

PDB ID : 1B7E  
Title : TRANSPOSASE INHIBITOR  
Authors : Davies, D.R.; Braam, L.M.; Reznikoff, W.S.; Rayment, I.  
Deposited on : 1999-01-22  
Resolution : 2.90 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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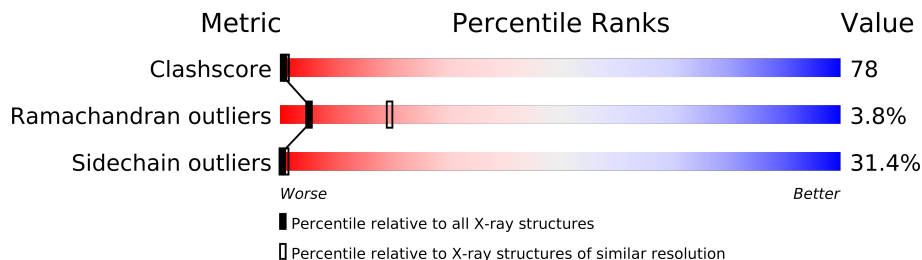
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.90 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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	420	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 2981 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.

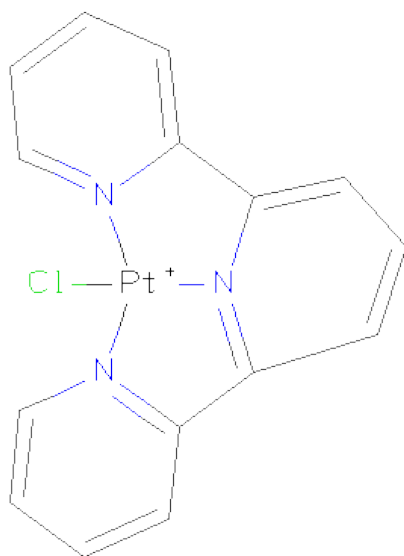
- Molecule 1 is a protein called PROTEIN (TRANSPOSASE INHIBITOR PROTEIN FROM TN5).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	372	2887	1832	518	527	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	GAP IN PDB ENTRY	GB 622948

- Molecule 2 is 2,2':6',2''-TERPYRIDINEPLATINUM(II) (three-letter code: TPT) (formula: C<sub>15</sub>H<sub>11</sub>ClN<sub>3</sub>Pt).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	Pt		
2	A	1	19	15	3	1	0	0
2	A	1	19	15	3	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		

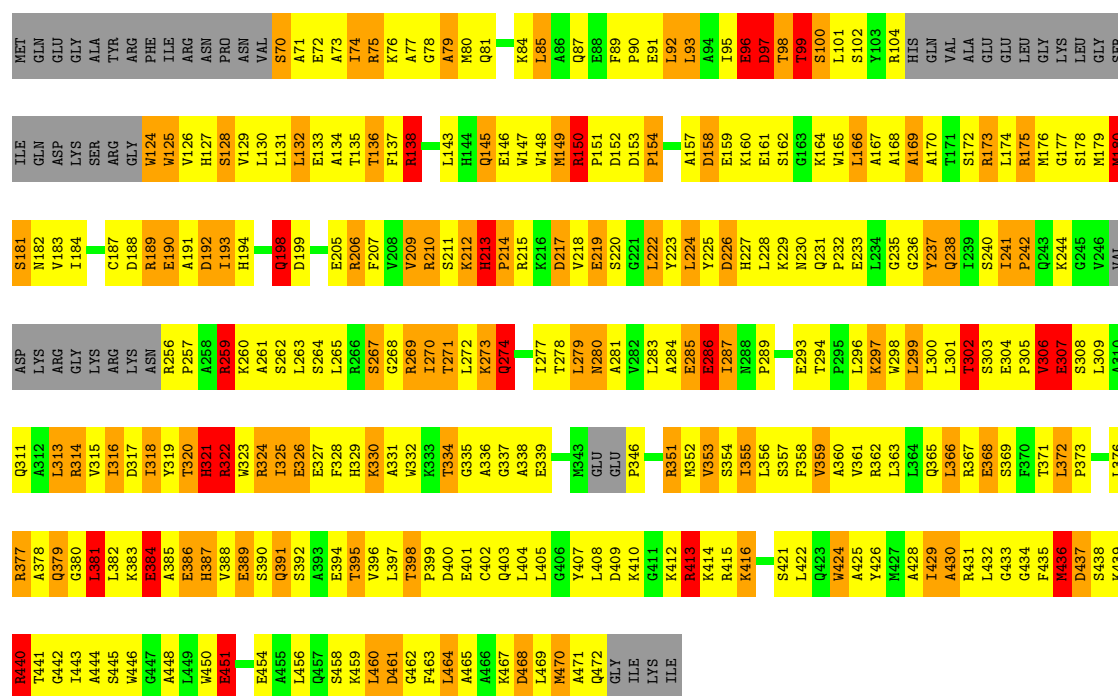
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (TRANSPOSASE INHIBITOR PROTEIN FROM TN5)

Chain A:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.80Å 71.90Å 41.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	94.3 (30.00-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPT

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	1.10	19/2945 (0.6%)	1.58	63/3985 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	GLU	CD-OE2	7.69	1.34	1.25
1	A	384	GLU	CD-OE1	7.55	1.33	1.25
1	A	368	GLU	CD-OE1	7.22	1.33	1.25
1	A	219	GLU	CD-OE1	7.20	1.33	1.25
1	A	339	GLU	CD-OE1	7.09	1.33	1.25
1	A	326	GLU	CD-OE2	7.08	1.33	1.25
1	A	451	GLU	CD-OE1	7.04	1.33	1.25
1	A	386	GLU	CD-OE1	6.91	1.33	1.25
1	A	389	GLU	CD-OE2	6.85	1.33	1.25
1	A	233	GLU	CD-OE1	6.82	1.33	1.25
1	A	161	GLU	CD-OE2	6.62	1.32	1.25
1	A	394	GLU	CD-OE2	6.52	1.32	1.25
1	A	327	GLU	CD-OE2	6.42	1.32	1.25
1	A	307	GLU	CD-OE2	5.96	1.32	1.25
1	A	454	GLU	CD-OE1	5.85	1.32	1.25
1	A	96	GLU	CD-OE2	5.50	1.31	1.25
1	A	285	GLU	CG-CD	-5.39	1.43	1.51
1	A	285	GLU	CD-OE2	5.21	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	GLU	CD-OE1	5.12	1.31	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	A	394	GLU	CB-CA-C	9.04	128.49	110.40
1	A	173	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	A	461	ASP	CB-CG-OD1	-8.62	110.54	118.30
1	A	188	ASP	CB-CG-OD1	-8.34	110.80	118.30
1	A	173	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	226	ASP	CB-CG-OD1	-7.94	111.15	118.30
1	A	351	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	A	322	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	169	ALA	CB-CA-C	-7.55	98.77	110.10
1	A	437	ASP	CB-CG-OD1	-7.55	111.51	118.30
1	A	138	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	A	150	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	A	79	ALA	CB-CA-C	-7.41	98.99	110.10
1	A	189	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	461	ASP	CB-CG-OD2	7.36	124.93	118.30
1	A	210	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	306	VAL	N-CA-CB	-6.94	96.22	111.50
1	A	415	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	A	223	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	A	188	ASP	CB-CA-C	-6.81	96.77	110.40
1	A	413	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	74	ILE	CB-CA-C	-6.76	98.07	111.60
1	A	199	ASP	CA-CB-CG	-6.76	98.54	113.40
1	A	97	ASP	CB-CG-OD1	-6.74	112.23	118.30
1	A	392	SER	N-CA-CB	6.74	120.61	110.50
1	A	322	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	217	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	75	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	A	217	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	A	99	THR	N-CA-CB	6.11	121.90	110.30
1	A	287	ILE	CB-CA-C	6.08	123.77	111.60
1	A	461	ASP	CA-CB-CG	-6.08	100.03	113.40
1	A	302	THR	CA-CB-CG2	-6.03	103.96	112.40
1	A	149	MET	CG-SD-CE	5.92	109.67	100.20
1	A	218	VAL	CB-CA-C	5.89	122.59	111.40
1	A	242	PRO	N-CA-CB	5.85	110.32	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	HIS	CA-CB-CG	5.78	123.42	113.60
1	A	199	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	131	LEU	N-CA-CB	-5.75	98.89	110.40
1	A	198	GLN	N-CA-CB	5.71	120.88	110.60
1	A	269	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	259	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	346	PRO	N-CA-CB	5.61	110.03	103.30
1	A	436	MET	CB-CA-C	5.53	121.45	110.40
1	A	191	ALA	N-CA-CB	5.52	117.83	110.10
1	A	209	VAL	CB-CA-C	-5.51	100.93	111.40
1	A	97	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	226	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	424	TRP	CA-CB-CG	-5.32	103.59	113.70
1	A	468	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	166	LEU	CB-CA-C	-5.17	100.38	110.20
1	A	430	ALA	N-CA-CB	5.16	117.32	110.10
1	A	463	PHE	N-CA-CB	-5.15	101.33	110.60
1	A	321	HIS	N-CA-CB	5.11	119.80	110.60
1	A	237	TYR	N-CA-CB	-5.11	101.41	110.60
1	A	440	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	468	ASP	N-CA-CB	5.09	119.76	110.60
1	A	209	VAL	CA-CB-CG1	-5.09	103.27	110.90
1	A	131	LEU	CB-CA-C	-5.08	100.54	110.20
1	A	175	ARG	CG-CD-NE	5.07	122.44	111.80
1	A	125	TRP	N-CA-CB	5.02	119.63	110.60
1	A	371	THR	CA-CB-CG2	-5.01	105.39	112.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	394	GLU	CA

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	2887	0	2850	453	1
2	A	38	0	22	16	0
3	A	56	0	0	10	0
All	All	2981	0	2872	453	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 78.

All (453) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:151:PRO:CG	1:A:157:ALA:HA	1.59	1.30
1:A:151:PRO:HG2	1:A:157:ALA:CA	1.69	1.20
1:A:153:ASP:OD1	1:A:154:PRO:HD2	1.42	1.17
1:A:151:PRO:HG2	1:A:157:ALA:CB	1.78	1.14
1:A:308:SER:H	1:A:311:GLN:NE2	1.46	1.13
1:A:73:ALA:HA	1:A:76:LYS:HD2	1.26	1.12
1:A:150:ARG:HD3	1:A:151:PRO:HD2	1.33	1.09
1:A:398:THR:HB	1:A:401:GLU:HG3	1.36	1.07
1:A:373:PRO:HD3	1:A:388:VAL:HG11	1.38	1.05
1:A:150:ARG:CD	1:A:151:PRO:HD2	1.87	1.03
1:A:98:THR:HA	1:A:127:HIS:HA	1.41	1.02
1:A:151:PRO:HG3	1:A:157:ALA:HA	1.41	0.99
1:A:402:CYS:SG	2:A:480:TPT:H1	2.03	0.99
1:A:137:PHE:O	1:A:324:ARG:NH2	1.97	0.97
1:A:330:LYS:HD3	1:A:446:TRP:HE1	1.27	0.96
1:A:267:SER:HB2	1:A:306:VAL:HG13	1.49	0.95
1:A:352:MET:HA	1:A:355:ILE:HG13	1.48	0.93
1:A:124:TRP:HB3	1:A:149:MET:HA	1.48	0.92
1:A:441:THR:HB	1:A:443:ILE:HD12	1.51	0.91
1:A:151:PRO:HG2	1:A:157:ALA:HA	1.27	0.91
1:A:308:SER:H	1:A:311:GLN:HE21	1.07	0.91
1:A:217:ASP:OD2	3:A:515:HOH:O	1.88	0.91
1:A:335:GLY:HA3	1:A:450:TRP:CE2	2.05	0.90
1:A:316:ILE:O	1:A:320:THR:HG23	1.73	0.89
1:A:398:THR:CB	1:A:401:GLU:HG3	2.02	0.89
1:A:332:TRP:HE1	1:A:357:SER:N	1.70	0.89
1:A:194:HIS:HD2	1:A:277:ILE:HD11	1.37	0.88
1:A:396:VAL:HG23	1:A:422:LEU:HD11	1.55	0.87
1:A:151:PRO:HG2	1:A:157:ALA:HB2	1.53	0.87
1:A:244:LYS:O	1:A:256:ARG:HD3	1.74	0.87
1:A:396:VAL:CG2	1:A:422:LEU:HD11	2.05	0.86
1:A:73:ALA:HA	1:A:76:LYS:CD	2.05	0.86
1:A:335:GLY:HA3	1:A:450:TRP:CD2	2.11	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:314:ARG:HH11	1:A:314:ARG:HG3	1.41	0.85
1:A:359:VAL:HG12	1:A:450:TRP:CH2	2.11	0.84
1:A:332:TRP:NE1	1:A:357:SER:N	2.25	0.84
1:A:369:SER:HB2	1:A:422:LEU:HD23	1.59	0.84
1:A:286:GLU:HG3	1:A:287:ILE:N	1.91	0.84
1:A:398:THR:HG22	1:A:401:GLU:H	1.42	0.84
1:A:194:HIS:CD2	1:A:277:ILE:HD11	2.12	0.84
1:A:272:LEU:HB3	1:A:274:GLN:HG2	1.58	0.83
1:A:317:ASP:O	1:A:320:THR:OG1	1.94	0.83
1:A:228:LEU:HD11	1:A:281:ALA:HB3	1.60	0.83
1:A:124:TRP:CB	1:A:149:MET:HA	2.07	0.82
1:A:332:TRP:CZ2	1:A:357:SER:HB3	2.14	0.82
1:A:398:THR:CG2	1:A:401:GLU:HG3	2.10	0.81
1:A:330:LYS:HD3	1:A:446:TRP:NE1	1.97	0.80
1:A:362:ARG:HA	1:A:365:GLN:CG	2.12	0.80
1:A:150:ARG:HD2	1:A:151:PRO:N	1.97	0.79
1:A:150:ARG:HD2	1:A:151:PRO:CD	2.12	0.79
1:A:308:SER:N	1:A:311:GLN:NE2	2.28	0.79
1:A:399:PRO:HB3	2:A:480:TPT:C14	2.13	0.79
1:A:271:THR:HA	1:A:278:THR:HA	1.65	0.79
1:A:404:LEU:HD23	1:A:460:LEU:HD12	1.65	0.79
1:A:362:ARG:HA	1:A:365:GLN:HG3	1.64	0.78
1:A:93:LEU:N	1:A:93:LEU:HD12	1.97	0.78
1:A:70:SER:O	1:A:74:ILE:HD12	1.83	0.78
1:A:150:ARG:CD	1:A:151:PRO:CD	2.61	0.78
1:A:398:THR:HB	1:A:401:GLU:CG	2.12	0.78
1:A:143:LEU:CD2	1:A:172:SER:HB3	2.15	0.77
1:A:270:ILE:N	1:A:279:LEU:O	2.17	0.76
1:A:361:VAL:O	1:A:365:GLN:HG2	1.84	0.76
1:A:99:THR:HG22	1:A:100:SER:H	1.51	0.76
1:A:147:TRP:CH2	1:A:353:VAL:HG11	2.21	0.75
1:A:376:LEU:HD12	1:A:385:ALA:HA	1.67	0.75
1:A:270:ILE:O	1:A:279:LEU:N	2.17	0.75
1:A:210:ARG:HB2	1:A:300:LEU:HD23	1.67	0.75
1:A:71:ALA:HA	1:A:74:ILE:CD1	2.15	0.75
1:A:153:ASP:OD1	1:A:154:PRO:CD	2.31	0.75
1:A:71:ALA:HA	1:A:74:ILE:HD13	1.68	0.74
1:A:267:SER:HB2	1:A:306:VAL:CG1	2.17	0.74
1:A:407:TYR:O	1:A:410:LYS:HG3	1.87	0.74
1:A:405:LEU:HD11	1:A:428:ALA:HB1	1.68	0.74
1:A:80:MET:HE2	1:A:175:ARG:HG2	1.70	0.73
1:A:399:PRO:HA	2:A:480:TPT:C15	2.18	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:LEU:HD11	1:A:281:ALA:CB	2.19	0.73
1:A:405:LEU:HD11	1:A:428:ALA:CB	2.18	0.73
1:A:435:PHE:CE1	1:A:444:ALA:HA	2.23	0.73
1:A:416:LYS:HD3	1:A:431:ARG:NH2	2.05	0.71
1:A:270:ILE:O	1:A:279:LEU:HD12	1.90	0.71
1:A:373:PRO:CD	1:A:388:VAL:HG11	2.19	0.71
1:A:190:GLU:O	1:A:213:HIS:NE2	2.23	0.71
1:A:264:SER:HB2	1:A:287:ILE:HD11	1.73	0.70
1:A:396:VAL:HG23	1:A:422:LEU:CD1	2.21	0.70
1:A:280:ASN:N	1:A:280:ASN:OD1	2.25	0.70
1:A:74:ILE:HG22	1:A:75:ARG:N	2.07	0.70
1:A:409:ASP:CG	1:A:412:LYS:HG3	2.11	0.70
1:A:148:TRP:CD2	1:A:164:LYS:HG3	2.27	0.70
1:A:385:ALA:O	1:A:389:GLU:HG2	1.93	0.69
1:A:133:GLU:O	1:A:137:PHE:HA	1.93	0.69
1:A:402:CYS:SG	2:A:480:TPT:C1	2.73	0.68
1:A:376:LEU:HD13	1:A:385:ALA:N	2.07	0.68
1:A:334:THR:HG22	1:A:335:GLY:N	2.07	0.68
1:A:80:MET:CE	1:A:175:ARG:HG2	2.23	0.68
1:A:399:PRO:O	1:A:403:GLN:HG3	1.93	0.68
1:A:222:LEU:HD22	1:A:226:ASP:HB3	1.75	0.67
1:A:283:LEU:HD12	1:A:298:TRP:O	1.95	0.67
1:A:76:LYS:O	1:A:80:MET:HG2	1.94	0.67
1:A:368:GLU:O	1:A:372:LEU:HB2	1.95	0.67
1:A:326:GLU:O	1:A:329:HIS:HB2	1.94	0.67
1:A:150:ARG:HD2	1:A:151:PRO:HD2	1.71	0.66
1:A:279:LEU:HD13	1:A:301:LEU:HD22	1.76	0.66
1:A:271:THR:HG23	1:A:278:THR:HB	1.78	0.66
1:A:70:SER:C	1:A:74:ILE:HD12	2.15	0.66
1:A:72:GLU:O	1:A:76:LYS:HG3	1.96	0.66
1:A:332:TRP:NE1	1:A:357:SER:CA	2.59	0.66
1:A:412:LYS:HB2	1:A:431:ARG:NH1	2.11	0.66
1:A:317:ASP:O	1:A:321:HIS:ND1	2.30	0.65
1:A:387:HIS:HA	1:A:390:SER:HG	1.62	0.65
1:A:173:ARG:NH2	1:A:205:GLU:OE1	2.30	0.65
1:A:151:PRO:CG	1:A:157:ALA:CA	2.37	0.65
1:A:469:LEU:CD1	1:A:469:LEU:N	2.60	0.65
1:A:127:HIS:HB3	1:A:146:GLU:HB3	1.79	0.64
1:A:99:THR:N	1:A:126:VAL:O	2.26	0.64
1:A:469:LEU:HD12	1:A:469:LEU:N	2.12	0.64
1:A:147:TRP:HH2	1:A:353:VAL:HG11	1.62	0.64
1:A:272:LEU:HB3	1:A:274:GLN:CG	2.25	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:LEU:HG	1:A:143:LEU:O	1.94	0.64
1:A:377:ARG:O	1:A:380:GLY:N	2.23	0.64
1:A:373:PRO:HD3	1:A:388:VAL:CG1	2.24	0.64
1:A:98:THR:OG1	1:A:148:TRP:HH2	1.81	0.64
1:A:297:LYS:NZ	1:A:297:LYS:CB	2.60	0.64
1:A:469:LEU:O	1:A:471:ALA:N	2.31	0.64
1:A:359:VAL:HG12	1:A:450:TRP:CZ3	2.33	0.64
1:A:259:ARG:NH2	1:A:286:GLU:OE1	2.31	0.63
1:A:387:HIS:HA	1:A:390:SER:OG	1.99	0.63
1:A:126:VAL:HA	1:A:146:GLU:O	1.98	0.63
1:A:314:ARG:O	1:A:318:ILE:HD12	1.99	0.62
1:A:388:VAL:HG12	1:A:389:GLU:N	2.09	0.62
1:A:270:ILE:HG22	1:A:279:LEU:CD1	2.28	0.62
1:A:213:HIS:CE1	2:A:481:TPT:C11	2.82	0.62
1:A:297:LYS:HZ2	1:A:297:LYS:HB2	1.63	0.62
1:A:78:GLY:O	1:A:81:GLN:HB2	1.99	0.62
1:A:127:HIS:CE1	1:A:165:TRP:CD2	2.87	0.62
1:A:224:LEU:N	1:A:224:LEU:HD13	2.13	0.62
1:A:398:THR:O	1:A:402:CYS:N	2.32	0.62
1:A:213:HIS:CE1	2:A:481:TPT:C10	2.83	0.62
1:A:137:PHE:CD1	1:A:321:HIS:CD2	2.87	0.61
1:A:353:VAL:HG12	1:A:354:SER:N	2.14	0.61
1:A:357:SER:OG	1:A:358:PHE:N	2.31	0.61
1:A:167:ALA:O	1:A:170:ALA:HB3	1.99	0.61
1:A:286:GLU:HG2	1:A:289:PRO:HB3	1.81	0.61
1:A:352:MET:CA	1:A:355:ILE:HG13	2.28	0.61
1:A:224:LEU:HD12	1:A:270:ILE:HD11	1.82	0.61
1:A:92:LEU:O	1:A:183:VAL:HA	2.01	0.61
1:A:398:THR:HG22	1:A:400:ASP:N	2.16	0.61
1:A:336:ALA:C	1:A:338:ALA:H	2.04	0.61
1:A:96:GLU:HG3	1:A:127:HIS:NE2	2.16	0.61
1:A:372:LEU:HB3	1:A:373:PRO:HD3	1.82	0.61
1:A:431:ARG:O	1:A:434:GLY:N	2.32	0.61
1:A:384:GLU:O	1:A:387:HIS:N	2.31	0.60
1:A:262:SER:HB2	3:A:504:HOH:O	2.00	0.60
1:A:305:PRO:O	1:A:306:VAL:HG23	2.02	0.60
1:A:330:LYS:NZ	3:A:552:HOH:O	2.35	0.60
1:A:164:LYS:O	1:A:167:ALA:HB3	2.02	0.60
1:A:362:ARG:O	1:A:366:LEU:HD12	2.02	0.60
1:A:376:LEU:CD1	1:A:385:ALA:HA	2.32	0.60
1:A:224:LEU:HD12	1:A:270:ILE:CD1	2.31	0.60
1:A:176:MET:CE	1:A:179:MET:HB3	2.32	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:242:PRO:HG2	1:A:323:TRP:CE2	2.36	0.59
1:A:74:ILE:O	1:A:77:ALA:HB3	2.03	0.59
1:A:319:TYR:O	1:A:322:ARG:N	2.35	0.59
1:A:95:ILE:N	1:A:130:LEU:O	2.34	0.59
1:A:179:MET:HE3	3:A:540:HOH:O	2.02	0.59
1:A:430:ALA:HB1	1:A:435:PHE:HB2	1.83	0.59
1:A:336:ALA:O	1:A:338:ALA:N	2.31	0.59
1:A:334:THR:HG22	1:A:450:TRP:CD1	2.38	0.59
1:A:442:GLY:C	1:A:443:ILE:HG13	2.22	0.58
1:A:416:LYS:HD3	1:A:431:ARG:HH22	1.68	0.58
1:A:97:ASP:O	1:A:128:SER:N	2.28	0.58
1:A:424:TRP:CZ3	2:A:480:TPT:H2	2.38	0.58
1:A:93:LEU:HD11	1:A:134:ALA:HA	1.85	0.58
1:A:136:THR:HG22	1:A:384:GLU:HB3	1.85	0.58
1:A:93:LEU:CD1	1:A:134:ALA:HB2	2.33	0.58
1:A:77:ALA:O	1:A:80:MET:HB2	2.03	0.58
1:A:217:ASP:HB2	1:A:270:ILE:HD11	1.86	0.58
1:A:465:ALA:O	1:A:469:LEU:HD13	2.04	0.58
1:A:174:LEU:HD23	1:A:174:LEU:C	2.24	0.58
1:A:270:ILE:O	1:A:278:THR:HA	2.04	0.57
1:A:369:SER:CB	1:A:422:LEU:HD23	2.32	0.57
1:A:398:THR:HG23	1:A:399:PRO:HD2	1.86	0.57
1:A:456:LEU:O	1:A:456:LEU:HG	1.99	0.57
1:A:373:PRO:HG3	1:A:388:VAL:CG1	2.34	0.57
1:A:93:LEU:HD11	1:A:134:ALA:CB	2.35	0.57
1:A:296:LEU:HD23	1:A:297:LYS:N	2.20	0.57
1:A:352:MET:HA	1:A:355:ILE:CG1	2.29	0.57
1:A:302:THR:OG1	1:A:303:SER:N	2.37	0.57
1:A:373:PRO:HG3	1:A:388:VAL:HG12	1.87	0.57
1:A:265:LEU:HD23	1:A:265:LEU:N	2.19	0.57
1:A:458:SER:O	1:A:461:ASP:N	2.38	0.57
1:A:143:LEU:HD21	1:A:172:SER:HA	1.87	0.56
1:A:305:PRO:C	1:A:306:VAL:HG23	2.25	0.56
1:A:177:GLY:O	1:A:180:MET:HB2	2.05	0.56
1:A:222:LEU:HD22	1:A:226:ASP:CB	2.35	0.56
1:A:412:LYS:CB	1:A:431:ARG:NH1	2.68	0.56
1:A:469:LEU:H	1:A:469:LEU:CD1	2.17	0.56
1:A:93:LEU:N	1:A:93:LEU:CD1	2.67	0.56
1:A:399:PRO:CB	2:A:480:TPT:C14	2.84	0.56
1:A:405:LEU:O	1:A:405:LEU:HD12	2.06	0.56
1:A:242:PRO:HG2	1:A:323:TRP:CZ2	2.40	0.56
1:A:308:SER:H	1:A:311:GLN:HE22	1.49	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:297:LYS:NZ	1:A:297:LYS:HB2	2.21	0.55
1:A:399:PRO:HB3	2:A:480:TPT:C13	2.37	0.55
1:A:151:PRO:CG	1:A:157:ALA:CB	2.70	0.55
1:A:125:TRP:CD1	1:A:125:TRP:N	2.75	0.55
1:A:237:TYR:O	1:A:263:LEU:N	2.34	0.55
1:A:296:LEU:HD11	1:A:298:TRP:CZ2	2.42	0.55
1:A:308:SER:N	1:A:311:GLN:HE21	1.91	0.55
1:A:270:ILE:HG22	1:A:279:LEU:HD12	1.88	0.54
1:A:438:SER:O	1:A:440:ARG:N	2.40	0.54
1:A:335:GLY:CA	1:A:450:TRP:CD2	2.87	0.54
1:A:91:GLU:C	1:A:92:LEU:HG	2.27	0.54
1:A:398:THR:CG2	1:A:400:ASP:H	2.20	0.54
1:A:332:TRP:HE1	1:A:356:LEU:C	2.10	0.54
1:A:93:LEU:HD11	1:A:134:ALA:CA	2.37	0.54
1:A:76:LYS:O	1:A:79:ALA:HB3	2.08	0.53
1:A:376:LEU:HB2	1:A:385:ALA:HB2	1.90	0.53
1:A:381:LEU:HB3	1:A:384:GLU:CD	2.29	0.53
1:A:213:HIS:CB	1:A:214:PRO:HD2	2.38	0.53
1:A:178:SER:O	1:A:181:SER:OG	2.25	0.53
1:A:176:MET:HE1	1:A:179:MET:HB3	1.89	0.53
1:A:331:ALA:O	1:A:450:TRP:NE1	2.36	0.53
1:A:127:HIS:CE1	1:A:165:TRP:CE2	2.96	0.53
1:A:261:ALA:HB1	1:A:286:GLU:OE2	2.08	0.53
1:A:225:TYR:CE1	1:A:283:LEU:HD21	2.43	0.53
1:A:356:LEU:O	1:A:360:ALA:N	2.42	0.53
1:A:213:HIS:CB	1:A:214:PRO:CD	2.87	0.53
1:A:367:ARG:NH2	1:A:446:TRP:CE2	2.77	0.53
1:A:353:VAL:CG1	1:A:354:SER:N	2.72	0.52
1:A:96:GLU:HG3	1:A:127:HIS:HE2	1.74	0.52
1:A:409:ASP:OD2	1:A:412:LYS:HG3	2.09	0.52
1:A:462:GLY:O	1:A:465:ALA:N	2.41	0.52
1:A:231:GLN:HB3	1:A:232:PRO:CD	2.39	0.52
1:A:190:GLU:HA	1:A:213:HIS:CE1	2.44	0.52
1:A:71:ALA:O	1:A:74:ILE:HB	2.09	0.52
1:A:332:TRP:NE1	1:A:357:SER:HA	2.23	0.52
1:A:137:PHE:CE2	1:A:321:HIS:NE2	2.78	0.52
1:A:399:PRO:HA	2:A:480:TPT:C14	2.39	0.52
1:A:372:LEU:CB	1:A:373:PRO:HD3	2.39	0.52
1:A:126:VAL:HG12	1:A:145:GLN:HG2	1.91	0.52
1:A:151:PRO:O	1:A:153:ASP:O	2.28	0.52
1:A:137:PHE:CZ	1:A:321:HIS:NE2	2.78	0.52
1:A:325:ILE:O	1:A:328:PHE:HB3	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:ASP:OD2	1:A:220:SER:HB2	2.09	0.52
1:A:438:SER:C	1:A:440:ARG:H	2.14	0.52
1:A:192:ASP:O	1:A:193:ILE:C	2.47	0.52
1:A:124:TRP:HB2	1:A:149:MET:HA	1.91	0.51
1:A:71:ALA:CA	1:A:74:ILE:CD1	2.86	0.51
1:A:226:ASP:O	1:A:230:ASN:ND2	2.44	0.51
1:A:224:LEU:HB3	1:A:299:LEU:HD11	1.92	0.51
1:A:460:LEU:HD23	1:A:464:LEU:CD2	2.41	0.51
1:A:359:VAL:CG1	1:A:450:TRP:CZ3	2.92	0.51
1:A:267:SER:CB	1:A:306:VAL:CG1	2.87	0.51
1:A:217:ASP:OD1	1:A:270:ILE:HD13	2.10	0.51
1:A:436:MET:HA	1:A:436:MET:HE3	1.93	0.51
1:A:194:HIS:HD2	1:A:277:ILE:CD1	2.16	0.51
1:A:263:LEU:HB3	1:A:265:LEU:HD21	1.93	0.51
1:A:460:LEU:CD2	1:A:464:LEU:HD22	2.40	0.51
1:A:462:GLY:O	1:A:465:ALA:HB3	2.11	0.51
1:A:179:MET:CE	1:A:182:ASN:ND2	2.74	0.51
1:A:149:MET:CE	1:A:152:ASP:OD1	2.58	0.51
1:A:98:THR:OG1	1:A:127:HIS:HB2	2.11	0.51
1:A:148:TRP:CE2	1:A:164:LYS:HG3	2.46	0.51
1:A:359:VAL:O	1:A:363:LEU:HG	2.11	0.51
1:A:377:ARG:O	1:A:379:GLN:N	2.43	0.51
1:A:229:LYS:NZ	1:A:285:GLU:OE2	2.44	0.51
1:A:384:GLU:CD	1:A:384:GLU:H	2.15	0.50
1:A:93:LEU:HD12	1:A:134:ALA:HB2	1.92	0.50
1:A:314:ARG:O	1:A:314:ARG:HD2	2.11	0.50
1:A:314:ARG:NH1	1:A:314:ARG:HG3	2.16	0.50
1:A:405:LEU:HD11	1:A:428:ALA:HB3	1.93	0.50
1:A:151:PRO:CB	1:A:157:ALA:HA	2.38	0.50
1:A:143:LEU:HD23	1:A:172:SER:HB3	1.90	0.50
1:A:132:LEU:N	1:A:132:LEU:CD1	2.74	0.50
1:A:373:PRO:CG	1:A:389:GLU:HB3	2.42	0.50
1:A:224:LEU:CB	1:A:299:LEU:HD11	2.42	0.50
1:A:71:ALA:CA	1:A:74:ILE:HD12	2.42	0.50
1:A:332:TRP:HZ2	1:A:353:VAL:O	1.95	0.50
1:A:241:ILE:HG12	1:A:242:PRO:HD2	1.94	0.50
1:A:362:ARG:HG2	1:A:365:GLN:HE21	1.77	0.49
1:A:334:THR:C	1:A:336:ALA:H	2.15	0.49
1:A:179:MET:SD	1:A:182:ASN:ND2	2.84	0.49
1:A:137:PHE:CG	1:A:321:HIS:CD2	3.00	0.49
1:A:268:GLY:O	1:A:280:ASN:HA	2.12	0.49
1:A:433:GLY:HA2	1:A:451:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:224:LEU:N	1:A:224:LEU:CD1	2.76	0.49
1:A:286:GLU:HG2	1:A:289:PRO:CB	2.42	0.49
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.66	0.49
1:A:398:THR:HG22	1:A:401:GLU:N	2.19	0.49
1:A:334:THR:C	1:A:336:ALA:N	2.66	0.49
1:A:179:MET:O	1:A:182:ASN:N	2.29	0.49
1:A:332:TRP:CZ2	1:A:353:VAL:HG13	2.48	0.48
1:A:405:LEU:HD22	1:A:429:ILE:HD11	1.94	0.48
1:A:181:SER:O	1:A:206:ARG:HD2	2.12	0.48
1:A:98:THR:CA	1:A:127:HIS:HA	2.30	0.48
1:A:428:ALA:O	1:A:431:ARG:HB2	2.14	0.48
1:A:263:LEU:HD23	1:A:286:GLU:HA	1.94	0.48
1:A:308:SER:O	1:A:311:GLN:N	2.47	0.48
1:A:99:THR:OG1	1:A:329:HIS:CE1	2.66	0.48
1:A:213:HIS:CD2	2:A:481:TPT:N3	2.82	0.48
1:A:355:ILE:O	1:A:358:PHE:N	2.47	0.47
1:A:404:LEU:O	1:A:404:LEU:HD12	2.14	0.47
1:A:409:ASP:OD1	1:A:409:ASP:O	2.31	0.47
1:A:231:GLN:HB3	1:A:232:PRO:HD2	1.95	0.47
1:A:96:GLU:HG2	1:A:96:GLU:O	2.12	0.47
1:A:376:LEU:CD1	1:A:385:ALA:CA	2.91	0.47
1:A:441:THR:HG21	3:A:507:HOH:O	2.13	0.47
1:A:262:SER:O	1:A:263:LEU:HD23	2.14	0.47
1:A:264:SER:CB	1:A:287:ILE:HD11	2.44	0.47
1:A:368:GLU:HG2	1:A:372:LEU:HG	1.95	0.47
1:A:125:TRP:O	1:A:147:TRP:HA	2.14	0.47
1:A:334:THR:O	1:A:336:ALA:N	2.48	0.47
1:A:75:ARG:NH2	3:A:521:HOH:O	2.44	0.47
1:A:469:LEU:HD13	1:A:469:LEU:H	1.78	0.47
1:A:381:LEU:HB3	1:A:384:GLU:OE1	2.14	0.47
1:A:127:HIS:HE1	1:A:165:TRP:CE2	2.32	0.47
1:A:222:LEU:HD13	1:A:227:HIS:HA	1.97	0.47
1:A:379:GLN:NE2	3:A:549:HOH:O	2.47	0.47
1:A:176:MET:HE1	1:A:179:MET:CB	2.43	0.47
1:A:401:GLU:HB3	1:A:456:LEU:HD21	1.96	0.47
1:A:328:PHE:HD2	1:A:329:HIS:CD2	2.33	0.47
1:A:332:TRP:CD1	1:A:357:SER:HA	2.50	0.47
1:A:362:ARG:HB3	1:A:396:VAL:CG1	2.44	0.47
1:A:318:ILE:HG22	1:A:319:TYR:N	2.30	0.47
1:A:383:LYS:O	1:A:386:GLU:HB2	2.15	0.47
1:A:165:TRP:O	1:A:168:ALA:N	2.48	0.46
1:A:150:ARG:CD	1:A:151:PRO:N	2.73	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:LEU:O	1:A:408:LEU:HG	2.15	0.46
1:A:213:HIS:HB3	1:A:214:PRO:HD2	1.97	0.46
1:A:273:LYS:HG2	1:A:273:LYS:H	1.40	0.46
1:A:314:ARG:HA	1:A:314:ARG:HD3	1.71	0.46
1:A:366:LEU:HD22	1:A:426:TYR:HA	1.97	0.46
1:A:184:ILE:HG22	1:A:207:PHE:HA	1.98	0.46
1:A:431:ARG:HA	1:A:435:PHE:H	1.80	0.46
1:A:147:TRP:CZ2	1:A:353:VAL:CG1	2.99	0.46
1:A:297:LYS:HB3	1:A:297:LYS:HZ3	1.81	0.46
1:A:160:LYS:O	1:A:164:LYS:HG2	2.16	0.46
1:A:143:LEU:HD21	1:A:172:SER:HB3	1.97	0.46
1:A:147:TRP:CH2	1:A:353:VAL:CG1	2.95	0.46
1:A:242:PRO:HG3	1:A:323:TRP:CD2	2.51	0.46
1:A:235:GLY:HA3	1:A:309:LEU:HD13	1.97	0.46
1:A:126:VAL:CG1	1:A:145:GLN:HG2	2.46	0.45
1:A:460:LEU:HD23	1:A:464:LEU:HD22	1.97	0.45
1:A:332:TRP:CZ2	1:A:353:VAL:O	2.69	0.45
1:A:408:LEU:HD13	1:A:432:LEU:HD21	1.98	0.45
1:A:469:LEU:C	1:A:471:ALA:N	2.68	0.45
1:A:365:GLN:O	1:A:422:LEU:HD21	2.17	0.45
1:A:89:PHE:HA	1:A:90:PRO:HD3	1.72	0.45
1:A:76:LYS:HG3	1:A:76:LYS:H	1.42	0.45
1:A:215:ARG:CB	1:A:224:LEU:HD21	2.45	0.45
1:A:176:MET:CE	1:A:179:MET:CB	2.93	0.45
1:A:206:ARG:O	1:A:207:PHE:HB3	2.16	0.45
1:A:421:SER:O	1:A:424:TRP:HB3	2.16	0.45
1:A:143:LEU:CD2	1:A:172:SER:CB	2.92	0.45
1:A:93:LEU:CD1	1:A:134:ALA:HA	2.45	0.45
1:A:213:HIS:NE2	2:A:481:TPT:C12	2.79	0.45
1:A:433:GLY:HA3	1:A:448:ALA:O	2.16	0.45
1:A:372:LEU:CB	1:A:373:PRO:CD	2.95	0.45
1:A:336:ALA:C	1:A:338:ALA:N	2.70	0.45
1:A:267:SER:HB2	1:A:306:VAL:O	2.16	0.45
1:A:279:LEU:HD13	1:A:301:LEU:CD2	2.45	0.45
1:A:307:GLU:CB	1:A:311:GLN:HE22	2.30	0.45
1:A:125:TRP:N	1:A:148:TRP:O	2.33	0.45
1:A:422:LEU:O	1:A:425:ALA:HB3	2.16	0.45
1:A:398:THR:CG2	1:A:401:GLU:H	2.23	0.45
1:A:100:SER:O	1:A:100:SER:OG	2.31	0.44
1:A:238:GLN:NE2	1:A:262:SER:OG	2.50	0.44
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.72	0.44
1:A:237:TYR:CZ	1:A:313:LEU:HG	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:227:HIS:HA	1:A:230:ASN:HD22	1.83	0.44
1:A:391:GLN:NE2	3:A:501:HOH:O	2.51	0.44
1:A:377:ARG:C	1:A:379:GLN:N	2.71	0.44
1:A:391:GLN:HG2	1:A:395:THR:HG21	1.99	0.44
1:A:284:ALA:O	1:A:297:LYS:HA	2.18	0.44
1:A:436:MET:HA	1:A:436:MET:CE	2.45	0.44
1:A:336:ALA:HA	1:A:356:LEU:HD23	2.00	0.44
1:A:435:PHE:CE2	1:A:437:ASP:HB2	2.53	0.44
1:A:85:LEU:HA	1:A:85:LEU:HD12	1.79	0.44
1:A:279:LEU:CD1	1:A:301:LEU:HD22	2.46	0.43
1:A:440:ARG:HG2	1:A:440:ARG:HH11	1.83	0.43
1:A:286:GLU:HG3	1:A:287:ILE:H	1.77	0.43
1:A:158:ASP:O	1:A:162:SER:HB2	2.18	0.43
1:A:408:LEU:HA	1:A:408:LEU:HD23	1.71	0.43
1:A:136:THR:O	1:A:137:PHE:HB2	2.19	0.43
1:A:359:VAL:HG12	1:A:450:TRP:HH2	1.79	0.43
1:A:440:ARG:HG2	1:A:440:ARG:NH1	2.33	0.43
1:A:271:THR:HA	1:A:277:ILE:O	2.18	0.43
1:A:242:PRO:CG	1:A:323:TRP:CD2	3.02	0.43
1:A:369:SER:OG	1:A:422:LEU:HB3	2.18	0.43
1:A:138:ARG:NH2	1:A:391:GLN:OE1	2.51	0.43
1:A:460:LEU:CD2	1:A:464:LEU:CD2	2.97	0.43
1:A:212:LYS:C	1:A:213:HIS:ND1	2.72	0.43
1:A:220:SER:C	1:A:222:LEU:N	2.72	0.43
1:A:405:LEU:CD1	1:A:428:ALA:HB1	2.45	0.43
1:A:281:ALA:HA	1:A:300:LEU:O	2.18	0.42
1:A:213:HIS:NE2	2:A:481:TPT:C11	2.82	0.42
1:A:373:PRO:CG	1:A:388:VAL:CG1	2.97	0.42
1:A:296:LEU:C	1:A:296:LEU:HD23	2.39	0.42
1:A:459:LYS:HG2	1:A:459:LYS:H	1.42	0.42
1:A:319:TYR:C	1:A:321:HIS:N	2.73	0.42
1:A:143:LEU:HD21	1:A:172:SER:CA	2.48	0.42
1:A:319:TYR:O	1:A:322:ARG:HB2	2.19	0.42
1:A:384:GLU:O	1:A:385:ALA:C	2.56	0.42
1:A:279:LEU:O	1:A:279:LEU:HD12	2.19	0.42
1:A:213:HIS:N	1:A:213:HIS:ND1	2.66	0.42
1:A:413:ARG:NH1	3:A:517:HOH:O	2.52	0.42
1:A:308:SER:OG	1:A:311:GLN:NE2	2.53	0.42
1:A:229:LYS:NZ	1:A:285:GLU:CD	2.73	0.42
1:A:93:LEU:CD1	1:A:134:ALA:CA	2.96	0.42
1:A:166:LEU:O	1:A:169:ALA:HB3	2.19	0.42
1:A:129:VAL:HG12	1:A:143:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:332:TRP:CE2	1:A:357:SER:CA	3.02	0.42
1:A:356:LEU:N	1:A:356:LEU:CD1	2.81	0.42
1:A:458:SER:O	1:A:460:LEU:N	2.52	0.42
1:A:386:GLU:O	1:A:390:SER:OG	2.36	0.41
1:A:313:LEU:N	1:A:313:LEU:HD13	2.34	0.41
1:A:213:HIS:ND1	2:A:481:TPT:C10	2.83	0.41
1:A:150:ARG:C	1:A:150:ARG:CD	2.89	0.41
1:A:311:GLN:HB2	1:A:311:GLN:HE21	1.62	0.41
1:A:325:ILE:HG21	1:A:325:ILE:HD12	1.71	0.41
1:A:334:THR:CG2	1:A:335:GLY:N	2.76	0.41
1:A:405:LEU:HD21	1:A:429:ILE:HG12	2.01	0.41
1:A:269:ARG:HA	1:A:280:ASN:HA	2.01	0.41
1:A:424:TRP:CH2	2:A:480:TPT:H2	2.55	0.41
1:A:209:VAL:HG12	1:A:209:VAL:O	2.04	0.41
1:A:168:ALA:O	1:A:172:SER:N	2.53	0.41
1:A:359:VAL:HG13	1:A:359:VAL:O	2.20	0.41
1:A:198:GLN:HB3	3:A:512:HOH:O	2.21	0.41
1:A:332:TRP:NE1	1:A:356:LEU:C	2.70	0.41
1:A:179:MET:CE	1:A:182:ASN:HD21	2.32	0.41
1:A:150:ARG:C	1:A:150:ARG:HD2	2.41	0.41
1:A:73:ALA:HA	1:A:76:LYS:CE	2.51	0.41
1:A:398:THR:CG2	1:A:400:ASP:N	2.80	0.41
1:A:267:SER:CB	1:A:306:VAL:O	2.68	0.41
1:A:306:VAL:CG1	1:A:306:VAL:O	2.69	0.41
1:A:224:LEU:HD12	1:A:270:ILE:HD12	2.03	0.41
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.48	0.41
1:A:296:LEU:HD11	1:A:298:TRP:CE2	2.56	0.41
1:A:438:SER:C	1:A:440:ARG:N	2.73	0.41
1:A:458:SER:C	1:A:460:LEU:N	2.73	0.41
1:A:87:GLN:C	1:A:89:PHE:H	2.24	0.41
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.72	0.40
1:A:313:LEU:C	1:A:315:VAL:N	2.74	0.40
1:A:404:LEU:HD12	1:A:408:LEU:HG	2.02	0.40
1:A:319:TYR:O	1:A:321:HIS:N	2.55	0.40
1:A:352:MET:O	1:A:355:ILE:CG1	2.69	0.40
1:A:236:GLY:HA2	1:A:263:LEU:O	2.20	0.40
1:A:213:HIS:CE1	2:A:481:TPT:C12	3.04	0.40
1:A:164:LYS:HA	1:A:164:LYS:HD3	1.62	0.40
1:A:303:SER:OG	1:A:304:GLU:HG2	2.21	0.40
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.79	0.40
1:A:376:LEU:CB	1:A:385:ALA:HB2	2.52	0.40
1:A:217:ASP:HB3	1:A:222:LEU:O	2.22	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:407:TYR:OH	1:A:468:ASP:OD2[2_665]	2.19	0.01

## 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	364/420 (87%)	274 (75%)	76 (21%)	14 (4%)	5	19

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	MET
1	A	154	PRO
1	A	274	GLN
1	A	378	ALA
1	A	439	LYS
1	A	306	VAL
1	A	384	GLU
1	A	180	MET
1	A	381	LEU
1	A	213	HIS
1	A	320	THR
1	A	337	GLY
1	A	257	PRO
1	A	214	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	290/349 (83%)	199 (69%)	91 (31%)	<b>0</b> <b>1</b>

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	84	LYS
1	A	85	LEU
1	A	92	LEU
1	A	93	LEU
1	A	96	GLU
1	A	97	ASP
1	A	98	THR
1	A	99	THR
1	A	100	SER
1	A	101	LEU
1	A	102	SER
1	A	104	ARG
1	A	124	TRP
1	A	128	SER
1	A	132	LEU
1	A	135	THR
1	A	136	THR
1	A	138	ARG
1	A	145	GLN
1	A	150	ARG
1	A	158	ASP
1	A	159	GLU
1	A	180	MET
1	A	181	SER
1	A	187	CYS
1	A	189	ARG
1	A	193	ILE
1	A	198	GLN
1	A	206	ARG
1	A	211	SER
1	A	212	LYS
1	A	213	HIS
1	A	219	GLU
1	A	222	LEU
1	A	224	LEU
1	A	238	GLN
1	A	240	SER

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Mol	Chain	Res	Type
1	A	241	ILE
1	A	259	ARG
1	A	260	LYS
1	A	267	SER
1	A	270	ILE
1	A	271	THR
1	A	273	LYS
1	A	274	GLN
1	A	279	LEU
1	A	280	ASN
1	A	286	GLU
1	A	293	GLU
1	A	294	THR
1	A	297	LYS
1	A	299	LEU
1	A	302	THR
1	A	307	GLU
1	A	313	LEU
1	A	314	ARG
1	A	316	ILE
1	A	318	ILE
1	A	321	HIS
1	A	322	ARG
1	A	324	ARG
1	A	325	ILE
1	A	330	LYS
1	A	334	THR
1	A	351	ARG
1	A	353	VAL
1	A	355	ILE
1	A	359	VAL
1	A	366	LEU
1	A	372	LEU
1	A	377	ARG
1	A	379	GLN
1	A	381	LEU
1	A	382	LEU
1	A	391	GLN
1	A	395	THR
1	A	398	THR
1	A	413	ARG
1	A	414	LYS

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Mol	Chain	Res	Type
1	A	416	LYS
1	A	429	ILE
1	A	436	MET
1	A	440	ARG
1	A	445	SER
1	A	451	GLU
1	A	460	LEU
1	A	464	LEU
1	A	467	LYS
1	A	470	MET
1	A	472	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	194	HIS
1	A	230	ASN
1	A	274	GLN
1	A	311	GLN
1	A	329	HIS
1	A	365	GLN
1	A	457	GLN
1	A	472	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are 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
2	TPT	A	480	1	20,23,24	1.01	1 (5%)	26,35,38	4.30	12 (46%)
2	TPT	A	481	-	20,23,24	1.60	4 (20%)	26,35,38	4.47	15 (57%)

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
2	TPT	A	480	1	-	0/0/20/26	0/0/5/5
2	TPT	A	481	-	-	0/0/20/26	0/0/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	481	TPT	C6-C5	3.87	1.57	1.47
2	A	481	TPT	C10-N2	2.97	1.42	1.36
2	A	480	TPT	C6-C5	2.28	1.53	1.47
2	A	481	TPT	C9-C10	-2.12	1.34	1.39
2	A	481	TPT	C3-C2	2.02	1.43	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	481	TPT	C10-C11-N3	12.68	132.72	114.94
2	A	480	TPT	C10-C11-N3	12.51	132.48	114.94
2	A	480	TPT	C9-C10-C11	11.09	146.76	123.76
2	A	481	TPT	C9-C10-C11	10.87	146.30	123.76
2	A	481	TPT	C11-C10-N2	-8.16	97.52	114.06
2	A	480	TPT	C11-C10-N2	-8.13	97.57	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	TPT	C12-C11-N3	-5.40	112.64	120.87
2	A	481	TPT	C2-C1-N1	-5.00	114.65	122.75
2	A	481	TPT	C12-C11-C10	-5.00	113.40	123.76
2	A	481	TPT	C12-C11-N3	-4.64	113.80	120.87
2	A	480	TPT	C12-C11-C10	-4.42	114.58	123.76
2	A	480	TPT	C15-N3-C11	4.21	128.68	118.71
2	A	481	TPT	C1-N1-C5	4.21	128.66	118.71
2	A	481	TPT	C6-C5-N1	4.05	120.61	114.94
2	A	481	TPT	C15-N3-C11	3.86	127.85	118.71
2	A	480	TPT	C14-C15-N3	-3.56	116.99	122.75
2	A	480	TPT	C2-C1-N1	-3.11	117.71	122.75
2	A	481	TPT	C14-C15-N3	-3.11	117.71	122.75
2	A	481	TPT	C4-C5-N1	-3.04	116.23	120.87
2	A	481	TPT	C10-N2-C6	2.96	127.90	123.07
2	A	480	TPT	C7-C6-N2	-2.82	115.39	120.29
2	A	480	TPT	C10-N2-C6	2.72	127.52	123.07
2	A	480	TPT	C9-C10-N2	-2.66	115.67	120.29
2	A	481	TPT	C7-C6-N2	-2.62	115.73	120.29
2	A	480	TPT	C6-C5-N1	2.44	118.35	114.94
2	A	481	TPT	C9-C10-N2	-2.43	116.06	120.29
2	A	481	TPT	C5-C6-N2	2.15	118.42	114.06

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.