



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:41 pm GMT

PDB ID : 1LPQ
Title : Human DNA Topoisomerase I (70 Kda) In Non-Covalent Complex With A 22
Base Pair DNA Duplex Containing an 8-oxoG Lesion
Authors : Leshner, D.T.; Pommier, Y.; Stewart, L.; Redinbo, M.R.
Deposited on : 2002-05-08
Resolution : 3.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

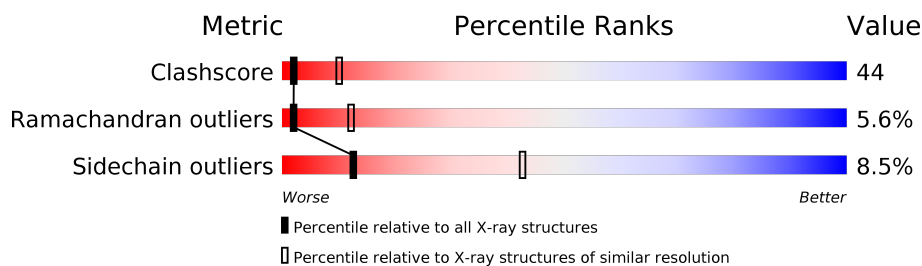
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	112137	1345 (3.18-3.10)
Ramachandran outliers	110173	1301 (3.18-3.10)
Sidechain outliers	110143	1301 (3.18-3.10)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	22	
2	C	22	
3	A	564	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5381 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 DNA chain called 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*TP*(8OG)P*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	22	Total	C	N	O	P	0	0	0
			454	219	87	127	21			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*CP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			443	217	71	134	21			

- Molecule 3 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	557	Total	C	N	O	S	0	0	0
			4457	2849	784	800	24			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PHE	TYR	ENGINEERED	UNP P11387

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	2	Total	O	0	0
			2	2		
4	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*TP*(8OG)P*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'

Chain B: 



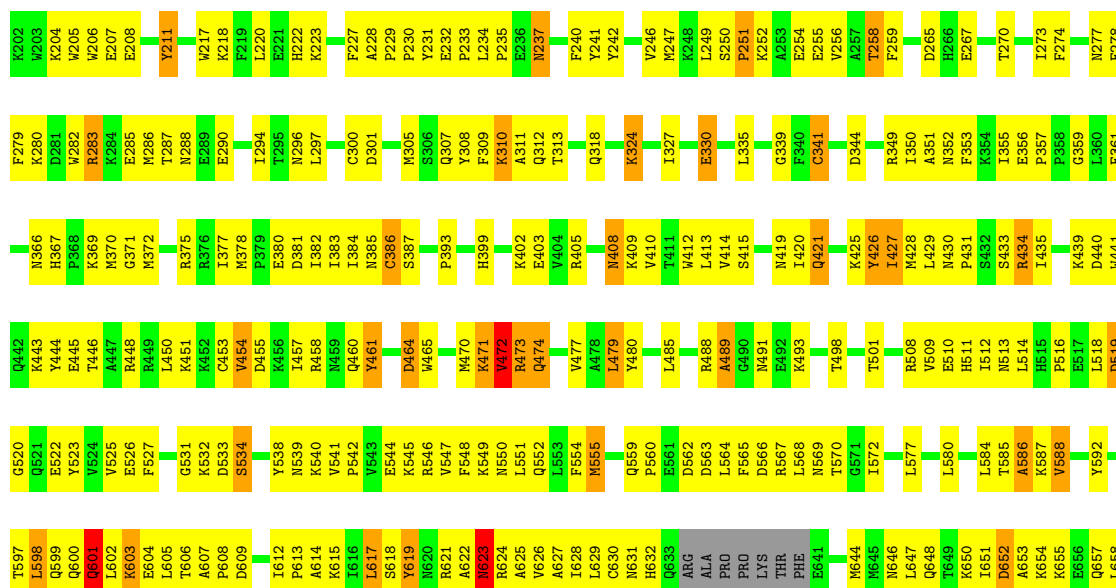
- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*CP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'

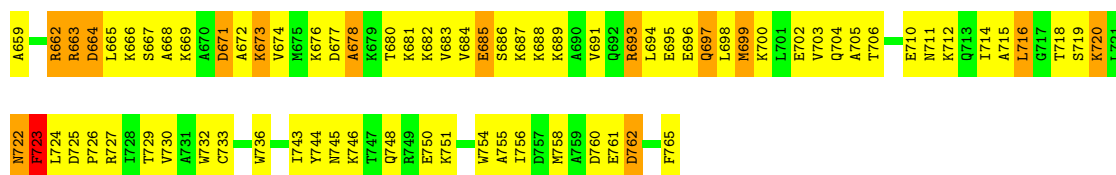
Chain C: 



- Molecule 3: DNA topoisomerase I

Chain A: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.20Å 122.50Å 72.00Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	19.87 – 3.14	Depositor
% Data completeness (in resolution range)	95.5 (19.87-3.14)	Depositor
R_{merge}	0.33	Depositor
R_{sym}	0.20	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.256 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5381	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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: 8OG

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	B	0.55	0/484	0.78	0/743
2	C	0.64	0/494	0.86	1/760 (0.1%)
3	A	0.45	0/4555	0.69	5/6142 (0.1%)
All	All	0.48	0/5533	0.71	6/7645 (0.1%)

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
2	C	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	664	ASP	N-CA-C	-7.79	89.98	111.00
3	A	472	VAL	N-CA-C	-6.99	92.12	111.00
3	A	426	TYR	N-CA-C	5.43	125.66	111.00
3	A	663	ARG	N-CA-C	-5.40	96.42	111.00
3	A	723	PHE	N-CA-C	5.26	125.19	111.00
2	C	112	DC	C1'-O4'-C4'	-5.01	105.09	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	112	DC	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	454	0	251	6	0
2	C	443	0	255	16	0
3	A	4457	0	4375	433	0
4	A	22	0	0	5	0
4	B	2	0	0	0	0
4	C	3	0	0	1	0
All	All	5381	0	4881	451	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 44.

All (451) 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)
3:A:473:ARG:CZ	3:A:550:ASN:HB3	1.64	1.26
3:A:473:ARG:NH2	3:A:550:ASN:HB3	1.57	1.17
3:A:473:ARG:CZ	3:A:550:ASN:CB	2.37	1.01
3:A:273:ILE:HD12	3:A:273:ILE:H	1.28	0.96
3:A:267:GLU:O	3:A:270:THR:HG22	1.68	0.91
3:A:664:ASP:C	3:A:666:LYS:H	1.75	0.90
3:A:283:ARG:HB3	4:A:1018:HOH:O	1.70	0.90
3:A:421:GLN:HA	3:A:421:GLN:HE21	1.35	0.90
3:A:241:TYR:HB2	3:A:301:ASP:HB3	1.54	0.90
3:A:617:LEU:HD13	3:A:703:VAL:HG22	1.54	0.89
3:A:628:ILE:HG13	3:A:714:ILE:HG21	1.54	0.89
3:A:618:SER:HA	3:A:621:ARG:HB3	1.56	0.87
3:A:654:LYS:HA	3:A:657:GLN:HG3	1.57	0.86
3:A:472:VAL:HG12	3:A:473:ARG:H	1.39	0.86
3:A:686:SER:HA	3:A:689:LYS:HG3	1.57	0.86
3:A:433:SER:HB3	3:A:435:ILE:HG22	1.58	0.85
3:A:408:ASN:HB2	3:A:409:LYS:NZ	1.92	0.85
3:A:252:LYS:HE2	3:A:285:GLU:OE1	1.77	0.85
3:A:659:ALA:HA	3:A:662:ARG:HB2	1.58	0.84
3:A:472:VAL:O	3:A:473:ARG:C	2.16	0.84
3:A:279:PHE:CD1	3:A:297:LEU:HB2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:TYR:CZ	3:A:545:LYS:HG3	2.14	0.82
3:A:508:ARG:HE	3:A:511:HIS:HE1	1.26	0.82
2:C:115:DG:H2'	2:C:116:DT:H72	1.62	0.81
3:A:585:THR:O	3:A:588:VAL:HG23	1.81	0.80
3:A:624:ARG:HD3	3:A:711:ASN:HB2	1.62	0.80
3:A:408:ASN:HB2	3:A:409:LYS:HZ2	1.47	0.80
3:A:473:ARG:CZ	3:A:550:ASN:CG	2.49	0.80
3:A:699:MET:HA	3:A:702:GLU:HG2	1.61	0.80
3:A:627:ALA:HB1	3:A:716:LEU:HB3	1.62	0.80
3:A:629:LEU:HB2	4:A:1006:HOH:O	1.81	0.79
3:A:598:LEU:HD21	3:A:623:ASN:HB2	1.64	0.79
1:B:7:DA:H2''	1:B:8:DC:H5''	1.65	0.79
3:A:655:LYS:O	3:A:658:LEU:HB3	1.83	0.78
3:A:516:PRO:O	3:A:522:GLU:HG3	1.83	0.78
3:A:601:GLN:HE21	3:A:601:GLN:HA	1.49	0.77
3:A:217:TRP:HZ3	3:A:387:SER:HB3	1.48	0.76
3:A:627:ALA:HB3	3:A:716:LEU:HD23	1.66	0.76
3:A:723:PHE:CE1	3:A:724:LEU:HG	2.21	0.76
3:A:380:GLU:O	3:A:402:LYS:HB2	1.85	0.76
3:A:470:MET:HE1	3:A:567:ARG:HG3	1.69	0.75
3:A:446:THR:HG22	3:A:588:VAL:HG11	1.68	0.75
3:A:745:ASN:ND2	3:A:748:GLN:HE21	1.84	0.75
3:A:473:ARG:NH2	3:A:550:ASN:CB	2.45	0.75
1:B:8:DC:H2'	1:B:9:DT:H72	1.69	0.74
3:A:426:TYR:O	3:A:427:ILE:HB	1.86	0.73
3:A:686:SER:HA	3:A:689:LYS:HE2	1.70	0.73
3:A:552:GLN:HA	3:A:555:MET:HG3	1.71	0.73
3:A:699:MET:HA	3:A:702:GLU:CG	2.18	0.73
3:A:444:TYR:O	3:A:448:ARG:HG3	1.89	0.72
3:A:430:ASN:OD1	3:A:431:PRO:HD2	1.89	0.72
2:C:106:DT:H2'	2:C:107:DT:H72	1.72	0.72
3:A:696:GLU:C	3:A:698:LEU:H	1.93	0.71
3:A:369:LYS:O	3:A:372:MET:HG3	1.89	0.71
3:A:235:PRO:HB2	3:A:237:ASN:ND2	2.05	0.71
3:A:617:LEU:CD1	3:A:703:VAL:HG22	2.21	0.70
3:A:621:ARG:CG	3:A:624:ARG:HH12	2.04	0.69
3:A:453:CYS:O	3:A:457:ILE:HG13	1.93	0.69
3:A:585:THR:H	3:A:588:VAL:CG2	2.05	0.69
3:A:719:SER:HA	3:A:723:PHE:CE2	2.27	0.69
3:A:297:LEU:HA	3:A:300:CYS:SG	2.33	0.69
3:A:250:SER:HB2	3:A:251:PRO:HD2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:510:GLU:HB3	3:A:560:PRO:HB3	1.75	0.68
3:A:730:VAL:HG11	3:A:756:ILE:HA	1.74	0.68
3:A:722:ASN:O	3:A:724:LEU:N	2.27	0.68
3:A:664:ASP:O	3:A:666:LYS:N	2.26	0.68
3:A:335:LEU:HD12	3:A:339:GLY:HA3	1.76	0.68
3:A:732:TRP:O	3:A:736:TRP:HD1	1.77	0.67
3:A:222:HIS:HE1	3:A:384:ILE:HG23	1.59	0.67
3:A:414:VAL:O	3:A:426:TYR:O	2.13	0.66
3:A:433:SER:CB	3:A:435:ILE:HG22	2.25	0.66
3:A:568:LEU:HA	3:A:572:ILE:HD12	1.77	0.66
3:A:222:HIS:CE1	3:A:384:ILE:HG23	2.31	0.66
2:C:115:DG:H2'	2:C:116:DT:C7	2.26	0.66
3:A:470:MET:CE	3:A:567:ARG:HG3	2.26	0.65
3:A:451:LYS:HA	3:A:592:TYR:CE1	2.31	0.65
3:A:211:TYR:OH	3:A:218:LYS:HB2	1.97	0.65
3:A:421:GLN:CA	3:A:421:GLN:HE21	2.08	0.65
3:A:552:GLN:O	3:A:555:MET:HB2	1.97	0.65
3:A:421:GLN:HA	3:A:421:GLN:NE2	2.10	0.65
3:A:448:ARG:HG2	3:A:765:PHE:CD1	2.31	0.65
2:C:109:DT:OP1	3:A:746:LYS:HD2	1.96	0.64
3:A:461:TYR:HA	3:A:464:ASP:CG	2.17	0.64
3:A:473:ARG:NE	3:A:550:ASN:CG	2.51	0.64
3:A:600:GLN:HA	3:A:603:LYS:HE2	1.80	0.64
3:A:665:LEU:HA	3:A:687:LYS:HG3	1.79	0.64
3:A:688:LYS:HA	3:A:691:VAL:HB	1.77	0.64
3:A:310:LYS:HG3	3:A:311:ALA:N	2.12	0.64
3:A:546:ARG:O	3:A:550:ASN:HB2	1.98	0.64
3:A:473:ARG:NH1	3:A:550:ASN:HB3	2.11	0.64
3:A:448:ARG:HG2	3:A:765:PHE:CE1	2.33	0.64
3:A:255:GLU:O	3:A:258:THR:CG2	2.46	0.64
3:A:408:ASN:HD22	3:A:408:ASN:N	1.93	0.64
3:A:460:GLN:O	3:A:464:ASP:OD1	2.16	0.64
3:A:664:ASP:C	3:A:666:LYS:N	2.47	0.64
3:A:621:ARG:NE	3:A:706:THR:HG21	2.13	0.63
3:A:489:ALA:HB1	3:A:570:THR:HG22	1.80	0.63
3:A:696:GLU:O	3:A:700:LYS:N	2.24	0.63
3:A:448:ARG:HD2	3:A:727:ARG:NH2	2.13	0.63
3:A:599:GLN:HE22	3:A:765:PHE:H	1.47	0.63
3:A:723:PHE:CD1	3:A:724:LEU:HG	2.34	0.63
3:A:493:LYS:NZ	3:A:501:THR:OG1	2.31	0.63
3:A:277:ASN:HA	3:A:280:LYS:NZ	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:351:ALA:HB2	3:A:429:LEU:O	1.99	0.63
3:A:754:TRP:O	3:A:758:MET:HG3	1.99	0.63
3:A:283:ARG:HA	3:A:286:MET:CE	2.29	0.62
3:A:598:LEU:CD2	3:A:623:ASN:HB2	2.29	0.62
2:C:106:DT:H2''	2:C:107:DT:C6	2.35	0.62
3:A:651:ILE:O	3:A:655:LYS:HB2	1.99	0.62
3:A:255:GLU:O	3:A:258:THR:HG23	1.99	0.62
3:A:601:GLN:O	3:A:604:GLU:HB3	1.99	0.62
3:A:601:GLN:HB3	3:A:622:ALA:HB1	1.81	0.62
3:A:566:ASP:O	3:A:567:ARG:HB2	2.00	0.61
3:A:509:VAL:CG2	3:A:560:PRO:HA	2.31	0.61
3:A:471:LYS:O	3:A:472:VAL:HB	2.01	0.61
3:A:523:TYR:OH	3:A:545:LYS:HG3	2.01	0.60
3:A:273:ILE:H	3:A:273:ILE:CD1	2.05	0.60
3:A:327:ILE:HA	3:A:330:GLU:HB2	1.83	0.60
3:A:696:GLU:CB	3:A:700:LYS:HE3	2.31	0.60
3:A:247:MET:HE1	3:A:294:ILE:HD11	1.83	0.60
3:A:619:TYR:HD2	3:A:619:TYR:C	2.05	0.60
3:A:696:GLU:O	3:A:698:LEU:N	2.34	0.60
3:A:473:ARG:NH2	3:A:550:ASN:C	2.54	0.60
3:A:282:TRP:O	3:A:286:MET:HG3	2.01	0.60
3:A:429:LEU:HD12	3:A:435:ILE:HG21	1.83	0.60
3:A:508:ARG:HE	3:A:511:HIS:CE1	2.15	0.60
3:A:450:LEU:O	3:A:454:VAL:HG12	2.02	0.60
3:A:678:ALA:O	3:A:682:LYS:HG2	2.01	0.60
3:A:431:PRO:HB3	3:A:751:LYS:HG3	1.83	0.60
3:A:472:VAL:HG12	3:A:473:ARG:N	2.14	0.60
3:A:663:ARG:O	3:A:664:ASP:CB	2.48	0.60
3:A:533:ASP:O	3:A:534:SER:HB2	2.02	0.60
3:A:568:LEU:HD13	3:A:568:LEU:C	2.22	0.60
3:A:434:ARG:HG2	3:A:434:ARG:O	2.02	0.59
3:A:659:ALA:CA	3:A:662:ARG:HB2	2.31	0.59
3:A:555:MET:HA	3:A:555:MET:HE3	1.84	0.59
3:A:658:LEU:HD21	4:A:1038:HOH:O	2.02	0.59
3:A:454:VAL:HG22	3:A:455:ASP:N	2.16	0.59
3:A:433:SER:C	3:A:435:ILE:H	2.05	0.59
3:A:602:LEU:C	3:A:604:GLU:H	2.04	0.59
3:A:696:GLU:C	3:A:698:LEU:N	2.55	0.59
3:A:222:HIS:HB3	3:A:341:CYS:HB2	1.84	0.59
3:A:356:GLU:OE2	3:A:425:LYS:NZ	2.36	0.59
3:A:477:VAL:O	3:A:480:TYR:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:465:TRP:O	3:A:473:ARG:HD3	2.03	0.59
3:A:617:LEU:HG	3:A:618:SER:N	2.18	0.58
3:A:220:LEU:HB3	3:A:386:CYS:HA	1.84	0.58
3:A:414:VAL:CG1	3:A:415:SER:N	2.65	0.58
3:A:621:ARG:HA	3:A:624:ARG:NH2	2.19	0.58
3:A:619:TYR:C	3:A:619:TYR:CD2	2.76	0.58
3:A:217:TRP:CZ3	3:A:387:SER:HB3	2.33	0.58
3:A:351:ALA:HB3	3:A:428:MET:O	2.04	0.58
3:A:628:ILE:HA	3:A:714:ILE:HG21	1.85	0.58
3:A:691:VAL:O	3:A:695:GLU:HG3	2.05	0.57
1:B:8:DC:H2'	1:B:9:DT:C7	2.33	0.57
3:A:621:ARG:HG3	3:A:624:ARG:HH12	1.67	0.57
3:A:694:LEU:HA	3:A:697:GLN:HB2	1.87	0.57
3:A:414:VAL:HG12	3:A:415:SER:N	2.19	0.57
3:A:429:LEU:HB3	3:A:433:SER:OG	2.04	0.57
3:A:614:ALA:O	3:A:617:LEU:HB3	2.04	0.57
3:A:628:ILE:HG13	3:A:714:ILE:HG13	1.86	0.57
3:A:665:LEU:HA	3:A:687:LYS:HD2	1.87	0.57
3:A:685:GLU:HG2	3:A:686:SER:N	2.16	0.57
3:A:508:ARG:HB2	3:A:511:HIS:CE1	2.40	0.56
3:A:668:ALA:HB1	3:A:684:VAL:HG22	1.87	0.56
3:A:568:LEU:HD13	3:A:569:ASN:N	2.20	0.56
3:A:671:ASP:C	3:A:673:LYS:H	2.08	0.56
3:A:231:TYR:CE2	3:A:233:PRO:HA	2.41	0.56
3:A:283:ARG:HA	3:A:286:MET:HE3	1.87	0.56
3:A:296:ASN:O	3:A:297:LEU:HB3	2.05	0.56
3:A:461:TYR:O	3:A:464:ASP:HB2	2.05	0.56
3:A:662:ARG:O	3:A:664:ASP:O	2.23	0.56
3:A:231:TYR:O	3:A:233:PRO:HD3	2.05	0.55
3:A:473:ARG:NE	3:A:550:ASN:OD1	2.38	0.55
3:A:369:LYS:HE3	3:A:421:GLN:HE22	1.70	0.55
3:A:597:THR:O	3:A:601:GLN:HG2	2.05	0.55
3:A:488:ARG:O	3:A:489:ALA:C	2.44	0.55
3:A:223:LYS:HA	3:A:393:PRO:HB3	1.89	0.55
3:A:648:GLN:O	3:A:652:ASP:HB2	2.07	0.55
3:A:217:TRP:CH2	3:A:408:ASN:ND2	2.74	0.55
3:A:665:LEU:HD12	3:A:687:LYS:HB3	1.89	0.55
3:A:231:TYR:CD1	3:A:255:GLU:HG3	2.43	0.54
3:A:367:HIS:HD2	3:A:369:LYS:H	1.54	0.54
3:A:509:VAL:HG22	3:A:560:PRO:HA	1.89	0.54
3:A:508:ARG:HB2	3:A:511:HIS:ND1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:606:THR:O	3:A:606:THR:HG22	2.06	0.54
3:A:686:SER:HA	3:A:689:LYS:CG	2.34	0.54
3:A:485:LEU:HD11	3:A:541:VAL:HG21	1.88	0.54
3:A:674:VAL:O	3:A:676:LYS:HG3	2.07	0.54
3:A:380:GLU:OE1	3:A:399:HIS:HD2	1.90	0.54
3:A:647:LEU:O	3:A:651:ILE:N	2.34	0.54
3:A:382:ILE:HG23	3:A:414:VAL:HG13	1.89	0.54
3:A:471:LYS:C	3:A:472:VAL:O	2.37	0.54
3:A:745:ASN:CG	3:A:748:GLN:HE21	2.11	0.54
3:A:234:LEU:HG	3:A:254:GLU:OE2	2.08	0.54
3:A:547:VAL:O	3:A:551:LEU:HB2	2.06	0.54
3:A:356:GLU:CD	3:A:425:LYS:HZ2	2.11	0.53
3:A:612:ILE:HB	3:A:613:PRO:HD3	1.89	0.53
3:A:231:TYR:HE2	3:A:233:PRO:HA	1.74	0.53
3:A:629:LEU:HD21	4:A:1008:HOH:O	2.08	0.53
3:A:665:LEU:HA	3:A:687:LYS:CG	2.37	0.53
1:B:11:8OG:H2"	1:B:11:8OG:O8	2.07	0.53
3:A:628:ILE:CG1	3:A:714:ILE:HG21	2.35	0.53
3:A:367:HIS:CD2	3:A:369:LYS:H	2.26	0.53
3:A:532:LYS:C	3:A:534:SER:H	2.11	0.53
3:A:683:VAL:O	3:A:687:LYS:HG2	2.09	0.53
3:A:686:SER:CA	3:A:689:LYS:HG3	2.35	0.53
3:A:693:ARG:HD3	3:A:694:LEU:HG	1.91	0.53
3:A:600:GLN:O	3:A:602:LEU:N	2.42	0.53
3:A:254:GLU:O	3:A:258:THR:HG22	2.09	0.52
3:A:733:CYS:SG	3:A:743:ILE:HD11	2.49	0.52
3:A:205:TRP:CG	3:A:434:ARG:HB2	2.44	0.52
3:A:585:THR:O	3:A:586:ALA:C	2.47	0.52
3:A:508:ARG:NE	3:A:511:HIS:HE1	2.01	0.52
3:A:431:PRO:HB3	3:A:751:LYS:CD	2.40	0.52
3:A:240:PHE:CD2	3:A:249:LEU:HD11	2.43	0.52
3:A:703:VAL:O	3:A:705:ALA:N	2.43	0.52
3:A:273:ILE:HG22	3:A:277:ASN:ND2	2.25	0.52
3:A:451:LYS:HA	3:A:592:TYR:HE1	1.74	0.52
2:C:115:DG:P	3:A:493:LYS:NZ	2.83	0.52
3:A:479:LEU:O	3:A:479:LEU:HD12	2.09	0.51
3:A:559:GLN:N	3:A:562:ASP:OD2	2.39	0.51
3:A:615:LYS:C	3:A:617:LEU:H	2.13	0.51
3:A:725:ASP:OD1	3:A:727:ARG:HG3	2.11	0.51
3:A:408:ASN:ND2	3:A:408:ASN:N	2.57	0.51
3:A:259:PHE:CD2	3:A:359:GLY:HA2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:622:ALA:C	3:A:624:ARG:H	2.14	0.51
3:A:361:PHE:HB2	3:A:420:ILE:CD1	2.40	0.51
3:A:746:LYS:O	3:A:750:GLU:HG3	2.10	0.51
3:A:382:ILE:HG22	3:A:383:ILE:N	2.25	0.51
3:A:726:PRO:HG2	3:A:755:ALA:CB	2.40	0.51
3:A:510:GLU:HB3	3:A:560:PRO:CB	2.40	0.51
3:A:615:LYS:C	3:A:617:LEU:N	2.62	0.51
3:A:686:SER:CA	3:A:689:LYS:HE2	2.39	0.51
3:A:722:ASN:H	3:A:722:ASN:HD22	1.58	0.51
3:A:242:TYR:CZ	3:A:294:ILE:HA	2.46	0.51
3:A:664:ASP:O	3:A:665:LEU:HB3	2.11	0.51
3:A:353:PHE:HD2	3:A:353:PHE:H	1.58	0.50
3:A:457:ILE:HG12	3:A:580:LEU:HD13	1.92	0.50
2:C:115:DG:H8	2:C:115:DG:H5'	1.75	0.50
3:A:698:LEU:O	3:A:702:GLU:HG2	2.11	0.50
3:A:726:PRO:O	3:A:730:VAL:HG23	2.11	0.50
3:A:413:LEU:HD23	3:A:413:LEU:N	2.26	0.50
3:A:501:THR:HB	3:A:531:GLY:O	2.12	0.50
3:A:513:ASN:O	3:A:514:LEU:HG	2.11	0.50
3:A:597:THR:O	3:A:600:GLN:HB3	2.12	0.50
3:A:691:VAL:O	3:A:695:GLU:CG	2.60	0.50
3:A:665:LEU:CA	3:A:687:LYS:HD2	2.41	0.50
3:A:703:VAL:C	3:A:705:ALA:N	2.63	0.50
3:A:237:ASN:HD22	3:A:237:ASN:C	2.13	0.50
3:A:686:SER:CB	3:A:689:LYS:HE2	2.42	0.50
3:A:727:ARG:HD3	3:A:754:TRP:HZ3	1.77	0.50
3:A:324:LYS:O	3:A:327:ILE:HG12	2.12	0.50
3:A:624:ARG:CD	3:A:711:ASN:HB2	2.39	0.49
3:A:703:VAL:O	3:A:706:THR:N	2.45	0.49
3:A:733:CYS:SG	3:A:743:ILE:CD1	3.00	0.49
3:A:309:PHE:O	3:A:312:GLN:HB3	2.12	0.49
3:A:663:ARG:C	3:A:664:ASP:O	2.45	0.49
3:A:622:ALA:O	3:A:624:ARG:N	2.45	0.49
3:A:632:HIS:O	3:A:715:ALA:N	2.45	0.49
1:B:8:DC:H2''	1:B:9:DT:C6	2.48	0.49
3:A:621:ARG:HA	3:A:624:ARG:CZ	2.43	0.49
3:A:628:ILE:HG13	3:A:714:ILE:CG2	2.35	0.49
3:A:430:ASN:O	3:A:433:SER:OG	2.23	0.49
3:A:255:GLU:O	3:A:258:THR:HG22	2.12	0.49
3:A:445:GLU:OE1	3:A:448:ARG:HD3	2.12	0.49
3:A:711:ASN:HD21	3:A:716:LEU:HD11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:512:ILE:HD11	3:A:564:LEU:CD2	2.42	0.49
2:C:115:DG:P	3:A:493:LYS:HZ3	2.36	0.49
3:A:686:SER:O	3:A:689:LYS:HB2	2.13	0.48
3:A:287:THR:HG23	3:A:290:GLU:OE1	2.14	0.48
3:A:665:LEU:HA	3:A:687:LYS:CD	2.42	0.48
3:A:431:PRO:HB3	3:A:751:LYS:CG	2.43	0.48
3:A:277:ASN:HA	3:A:280:LYS:HZ2	1.77	0.48
3:A:375:ARG:HG3	3:A:419:ASN:ND2	2.28	0.48
2:C:103:DA:H2''	2:C:104:DA:OP2	2.12	0.48
3:A:471:LYS:O	3:A:472:VAL:C	2.47	0.48
3:A:654:LYS:O	3:A:657:GLN:HB2	2.13	0.48
3:A:624:ARG:HD3	3:A:710:GLU:O	2.13	0.48
3:A:458:ARG:C	3:A:460:GLN:N	2.66	0.48
3:A:522:GLU:HG2	3:A:523:TYR:CD1	2.49	0.48
3:A:622:ALA:C	3:A:624:ARG:N	2.66	0.48
3:A:440:ASP:O	3:A:443:LYS:HB3	2.14	0.48
3:A:465:TRP:O	3:A:473:ARG:CD	2.61	0.48
3:A:648:GLN:C	3:A:650:LYS:H	2.17	0.48
2:C:106:DT:H2'	2:C:107:DT:C7	2.41	0.48
3:A:621:ARG:HA	3:A:624:ARG:NH1	2.29	0.47
3:A:665:LEU:O	3:A:668:ALA:HB3	2.14	0.47
3:A:685:GLU:O	3:A:689:LYS:HG3	2.14	0.47
3:A:274:PHE:CE1	3:A:371:GLY:HA2	2.48	0.47
3:A:310:LYS:O	3:A:313:THR:N	2.47	0.47
3:A:335:LEU:HD12	3:A:335:LEU:O	2.15	0.47
3:A:518:LEU:O	3:A:520:GLY:N	2.47	0.47
3:A:654:LYS:CA	3:A:657:GLN:HG3	2.38	0.47
3:A:658:LEU:HD11	3:A:662:ARG:NH1	2.30	0.47
3:A:695:GLU:O	3:A:698:LEU:HB3	2.14	0.47
3:A:410:VAL:HB	3:A:412:TRP:CD1	2.50	0.47
3:A:509:VAL:HB	3:A:555:MET:HE1	1.96	0.47
3:A:241:TYR:CE2	3:A:246:VAL:HG22	2.50	0.47
3:A:527:PHE:O	3:A:538:TYR:HA	2.15	0.47
3:A:686:SER:HA	3:A:689:LYS:CE	2.44	0.47
3:A:533:ASP:O	3:A:534:SER:CB	2.62	0.47
3:A:663:ARG:O	3:A:664:ASP:HB2	2.15	0.47
3:A:703:VAL:C	3:A:705:ALA:H	2.18	0.47
3:A:585:THR:H	3:A:588:VAL:HG23	1.79	0.47
3:A:699:MET:HA	3:A:702:GLU:HG3	1.96	0.47
3:A:720:LYS:HB2	3:A:720:LYS:HE3	1.61	0.47
3:A:682:LYS:HA	3:A:685:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:601:GLN:O	3:A:605:LEU:HD12	2.16	0.46
3:A:235:PRO:HB2	3:A:237:ASN:HD21	1.78	0.46
3:A:297:LEU:HD13	3:A:297:LEU:O	2.15	0.46
3:A:650:LYS:O	3:A:653:ALA:HB3	2.15	0.46
3:A:220:LEU:O	3:A:386:CYS:HB2	2.15	0.46
3:A:585:THR:O	3:A:587:LYS:N	2.48	0.46
3:A:632:HIS:CE1	3:A:718:THR:HG1	2.34	0.46
3:A:723:PHE:CD1	3:A:723:PHE:C	2.88	0.46
3:A:604:GLU:HB3	3:A:605:LEU:HD12	1.98	0.46
3:A:632:HIS:CE1	3:A:718:THR:OG1	2.68	0.46
3:A:246:VAL:HG12	3:A:247:MET:N	2.30	0.46
3:A:699:MET:CA	3:A:702:GLU:HG2	2.40	0.46
3:A:283:ARG:O	3:A:286:MET:HB2	2.15	0.46
3:A:651:ILE:O	3:A:655:LYS:CB	2.63	0.46
3:A:555:MET:HA	3:A:555:MET:CE	2.44	0.46
3:A:619:TYR:OH	3:A:729:THR:CG2	2.64	0.46
3:A:434:ARG:O	3:A:434:ARG:CG	2.63	0.45
3:A:548:PHE:C	3:A:548:PHE:CD2	2.89	0.45
3:A:473:ARG:HH21	3:A:550:ASN:C	2.19	0.45
3:A:621:ARG:HA	3:A:624:ARG:HH22	1.80	0.45
3:A:565:PHE:O	3:A:568:LEU:HB3	2.16	0.45
3:A:615:LYS:O	3:A:617:LEU:N	2.49	0.45
3:A:429:LEU:HD12	3:A:435:ILE:CG2	2.45	0.45
3:A:644:MET:C	3:A:646:ASN:H	2.20	0.45
3:A:485:LEU:CD1	3:A:541:VAL:HG21	2.47	0.45
3:A:512:ILE:HD11	3:A:564:LEU:HD22	1.97	0.45
3:A:680:THR:C	3:A:682:LYS:H	2.18	0.45
3:A:470:MET:O	3:A:473:ARG:O	2.35	0.45
3:A:600:GLN:O	3:A:601:GLN:C	2.55	0.45
3:A:673:LYS:HB3	3:A:674:VAL:H	1.48	0.45
3:A:247:MET:CE	3:A:294:ILE:HD11	2.46	0.45
3:A:369:LYS:O	3:A:370:MET:C	2.55	0.45
3:A:665:LEU:CD1	3:A:687:LYS:HB3	2.47	0.45
3:A:217:TRP:O	3:A:408:ASN:HB3	2.17	0.45
3:A:385:ASN:HD21	3:A:410:VAL:CG2	2.28	0.45
3:A:457:ILE:HG23	3:A:580:LEU:CD1	2.47	0.45
3:A:667:SER:O	3:A:671:ASP:HB2	2.17	0.45
2:C:113:DA:H2"	2:C:114:DA:H8	1.82	0.45
3:A:545:LYS:HD3	3:A:549:LYS:HZ1	1.81	0.45
3:A:231:TYR:CE1	3:A:255:GLU:HA	2.53	0.44
3:A:668:ALA:HB2	3:A:687:LYS:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:514:LEU:CD2	3:A:525:VAL:HG22	2.47	0.44
3:A:378:MET:C	3:A:380:GLU:N	2.71	0.44
3:A:677:ASP:CG	3:A:678:ALA:H	2.21	0.44
3:A:310:LYS:HE3	3:A:310:LYS:O	2.17	0.44
3:A:355:ILE:CG2	3:A:356:GLU:N	2.81	0.44
3:A:628:ILE:C	3:A:630:CYS:H	2.21	0.44
3:A:669:LYS:HD2	3:A:669:LYS:N	2.32	0.44
3:A:732:TRP:O	3:A:736:TRP:CD1	2.65	0.44
3:A:431:PRO:CB	3:A:751:LYS:HG3	2.48	0.44
3:A:283:ARG:HG3	3:A:286:MET:HE3	1.99	0.44
3:A:378:MET:O	3:A:380:GLU:N	2.50	0.44
3:A:523:TYR:O	3:A:542:PRO:HA	2.17	0.44
3:A:441:TRP:CD2	4:A:1005:HOH:O	2.69	0.44
3:A:256:VAL:HG21	3:A:285:GLU:HG3	1.99	0.44
3:A:355:ILE:HG22	3:A:356:GLU:N	2.32	0.44
3:A:687:LYS:HA	3:A:687:LYS:HD3	1.70	0.44
3:A:403:GLU:OE1	3:A:405:ARG:HB3	2.18	0.44
3:A:446:THR:HG22	3:A:588:VAL:CG1	2.43	0.44
3:A:523:TYR:HD2	3:A:548:PHE:CG	2.36	0.44
3:A:513:ASN:HB3	3:A:526:GLU:HB3	1.99	0.44
3:A:597:THR:HA	3:A:600:GLN:HB3	2.00	0.44
3:A:544:GLU:HB2	3:A:547:VAL:HG23	1.99	0.43
3:A:237:ASN:ND2	3:A:237:ASN:C	2.72	0.43
3:A:246:VAL:CG1	3:A:247:MET:N	2.80	0.43
3:A:433:SER:C	3:A:435:ILE:N	2.70	0.43
3:A:349:ARG:HG3	3:A:430:ASN:HB2	1.99	0.43
3:A:694:LEU:O	3:A:697:GLN:N	2.51	0.43
3:A:205:TRP:O	3:A:208:GLU:HB2	2.18	0.43
4:C:1003:HOH:O	3:A:352:ASN:HB2	2.18	0.43
3:A:448:ARG:O	3:A:451:LYS:HB3	2.18	0.43
3:A:577:LEU:HB3	3:A:584:LEU:HD23	2.00	0.43
3:A:722:ASN:ND2	3:A:722:ASN:H	2.17	0.43
3:A:458:ARG:C	3:A:460:GLN:H	2.22	0.43
1:B:21:DT:H5"	3:A:650:LYS:HE2	2.00	0.43
2:C:115:DG:H2"	2:C:116:DT:C6	2.53	0.43
3:A:356:GLU:HA	3:A:357:PRO:HD3	1.93	0.43
3:A:625:ALA:HA	3:A:628:ILE:HG22	2.01	0.43
3:A:351:ALA:CB	3:A:428:MET:O	2.66	0.43
3:A:472:VAL:O	3:A:474:GLN:N	2.52	0.43
3:A:597:THR:HG21	3:A:626:VAL:HG22	2.01	0.43
3:A:732:TRP:CE3	3:A:733:CYS:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:628:ILE:C	3:A:630:CYS:N	2.72	0.43
3:A:367:HIS:CE1	3:A:498:THR:HA	2.54	0.42
3:A:518:LEU:O	3:A:519:ASP:C	2.57	0.42
3:A:339:GLY:O	3:A:349:ARG:HD3	2.19	0.42
3:A:736:TRP:N	3:A:736:TRP:CD1	2.88	0.42
2:C:113:DA:H2"	2:C:114:DA:C8	2.53	0.42
3:A:451:LYS:HG2	3:A:592:TYR:HE1	1.84	0.42
3:A:662:ARG:C	3:A:663:ARG:O	2.54	0.42
3:A:305:MET:O	3:A:308:TYR:HB3	2.19	0.42
3:A:353:PHE:CD2	3:A:353:PHE:N	2.86	0.42
3:A:621:ARG:O	3:A:624:ARG:CB	2.68	0.42
3:A:282:TRP:CZ3	3:A:297:LEU:HD23	2.54	0.42
3:A:427:ILE:HG22	3:A:427:ILE:O	2.17	0.42
3:A:532:LYS:O	3:A:533:ASP:HB2	2.19	0.42
3:A:617:LEU:CG	3:A:618:SER:N	2.82	0.42
3:A:204:LYS:HG2	3:A:206:TRP:CZ2	2.54	0.42
3:A:408:ASN:HB2	3:A:409:LYS:HZ3	1.81	0.42
3:A:526:GLU:HA	3:A:540:LYS:HA	2.01	0.42
3:A:629:LEU:C	3:A:629:LEU:HD12	2.40	0.42
3:A:682:LYS:O	3:A:685:GLU:OE1	2.37	0.42
3:A:628:ILE:CD1	3:A:714:ILE:HG13	2.50	0.42
3:A:229:PRO:HA	3:A:230:PRO:HD3	1.89	0.42
3:A:602:LEU:C	3:A:604:GLU:N	2.71	0.42
2:C:109:DT:H2"	2:C:110:DT:OP2	2.19	0.42
3:A:607:ALA:HA	3:A:608:PRO:HD3	1.92	0.42
3:A:204:LYS:HB3	3:A:207:GLU:HG3	2.02	0.42
3:A:644:MET:C	3:A:646:ASN:N	2.71	0.42
3:A:662:ARG:O	3:A:665:LEU:HB3	2.20	0.42
3:A:282:TRP:HZ3	3:A:297:LEU:HD23	1.84	0.41
3:A:491:ASN:ND2	3:A:570:THR:HG21	2.35	0.41
3:A:719:SER:HA	3:A:723:PHE:CZ	2.55	0.41
3:A:568:LEU:HA	3:A:572:ILE:CD1	2.48	0.41
3:A:722:ASN:ND2	3:A:722:ASN:N	2.68	0.41
3:A:518:LEU:HG	3:A:519:ASP:N	2.35	0.41
3:A:598:LEU:HD22	3:A:598:LEU:HA	1.95	0.41
3:A:659:ALA:HA	3:A:662:ARG:CB	2.41	0.41
3:A:668:ALA:HB1	3:A:684:VAL:HG13	2.01	0.41
3:A:744:TYR:HB3	3:A:748:GLN:HB2	2.01	0.41
3:A:277:ASN:HA	3:A:280:LYS:HZ3	1.86	0.41
3:A:350:ILE:HG21	3:A:353:PHE:HB3	2.03	0.41
3:A:760:ASP:C	3:A:762:ASP:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:443:LYS:HE2	3:A:444:TYR:CZ	2.55	0.41
3:A:369:LYS:HE3	3:A:421:GLN:NE2	2.35	0.41
3:A:532:LYS:C	3:A:534:SER:N	2.72	0.41
3:A:730:VAL:HG11	3:A:755:ALA:O	2.21	0.41
3:A:664:ASP:CG	3:A:687:LYS:HZ1	2.22	0.41
3:A:445:GLU:O	3:A:448:ARG:N	2.53	0.41
3:A:627:ALA:CB	3:A:716:LEU:HB3	2.40	0.41
3:A:256:VAL:HG12	3:A:278:PHE:CE1	2.56	0.41
3:A:488:ARG:HG3	3:A:488:ARG:HH11	1.86	0.41
3:A:621:ARG:O	3:A:624:ARG:NH1	2.54	0.40
3:A:228:ALA:HB1	3:A:229:PRO:HD2	2.02	0.40
3:A:377:ILE:HG23	3:A:381:ASP:HB2	2.04	0.40
3:A:686:SER:HB2	3:A:689:LYS:HE2	2.03	0.40
3:A:711:ASN:HD21	3:A:716:LEU:CD1	2.34	0.40
3:A:732:TRP:CE3	3:A:733:CYS:N	2.90	0.40
3:A:745:ASN:OD1	3:A:745:ASN:C	2.59	0.40
2:C:108:DT:H1'	2:C:109:DT:H5'	2.03	0.40
3:A:240:PHE:CG	3:A:241:TYR:N	2.89	0.40
3:A:612:ILE:HD13	3:A:612:ILE:HA	1.99	0.40
2:C:119:DT:H2'	2:C:120:DT:H72	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	553/564 (98%)	412 (74%)	110 (20%)	31 (6%)	2 12

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	386	CYS

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Mol	Chain	Res	Type
3	A	473	ARG
3	A	519	ASP
3	A	673	LYS
3	A	723	PHE
3	A	427	ILE
3	A	472	VAL
3	A	474	GLN
3	A	586	ALA
3	A	601	GLN
3	A	609	ASP
3	A	617	LEU
3	A	678	ALA
3	A	697	GLN
3	A	318	GLN
3	A	344	ASP
3	A	489	ALA
3	A	539	ASN
3	A	603	LYS
3	A	623	ASN
3	A	681	LYS
3	A	704	GLN
3	A	366	ASN
3	A	534	SER
3	A	672	ALA
3	A	712	LYS
3	A	720	LYS
3	A	227	PHE
3	A	324	LYS
3	A	251	PRO
3	A	471	LYS

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	
3	A	457/508 (90%)	418 (92%)	39 (8%)	12	42

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	211	TYR
3	A	232	GLU
3	A	237	ASN
3	A	258	THR
3	A	265	ASP
3	A	283	ARG
3	A	288	ASN
3	A	307	GLN
3	A	310	LYS
3	A	330	GLU
3	A	341	CYS
3	A	408	ASN
3	A	421	GLN
3	A	434	ARG
3	A	439	LYS
3	A	454	VAL
3	A	461	TYR
3	A	464	ASP
3	A	479	LEU
3	A	554	PHE
3	A	555	MET
3	A	563	ASP
3	A	588	VAL
3	A	598	LEU
3	A	601	GLN
3	A	619	TYR
3	A	623	ASN
3	A	631	ASN
3	A	652	ASP
3	A	662	ARG
3	A	671	ASP
3	A	685	GLU
3	A	693	ARG
3	A	699	MET
3	A	716	LEU
3	A	722	ASN
3	A	723	PHE
3	A	761	GLU
3	A	762	ASP

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

Mol	Chain	Res	Type
3	A	237	ASN
3	A	288	ASN
3	A	307	GLN
3	A	346	HIS
3	A	367	HIS
3	A	385	ASN
3	A	399	HIS
3	A	406	HIS
3	A	408	ASN
3	A	421	GLN
3	A	474	GLN
3	A	511	HIS
3	A	599	GLN
3	A	601	GLN
3	A	632	HIS
3	A	697	GLN
3	A	722	ASN
3	A	748	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	8OG	B	11	1,2	17,25,26	1.28	2 (11%)	22,37,40	2.45	5 (22%)

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	8OG	B	11	1,2	-	0/3/21/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	8OG	C8-N7	-3.21	1.30	1.34
1	B	11	8OG	C6-N1	3.65	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	8OG	C5-C6-N1	-8.32	111.63	123.48
1	B	11	8OG	C2-N3-C4	-2.93	111.74	115.16
1	B	11	8OG	N3-C2-N1	-2.37	124.00	127.46
1	B	11	8OG	C6-C5-C4	-2.03	118.83	120.84
1	B	11	8OG	C6-N1-C2	6.20	124.98	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	11	8OG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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.