



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:45 am BST

PDB ID : 2OGZ
Title : Crystal structure of DPP-IV complexed with Lilly aryl ketone inhibitor
Authors : Timm, D.E.
Deposited on : 2007-01-09
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

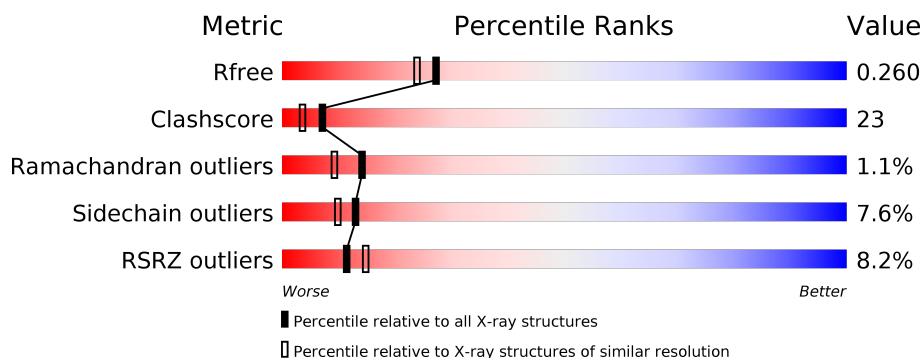
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>9%</div> <div>61%</div> <div>34%</div> <div>5%</div> </div>
1	B	728	<div> <div>7%</div> <div>61%</div> <div>34%</div> <div>5%</div> </div>

2 Entry composition [i](#)

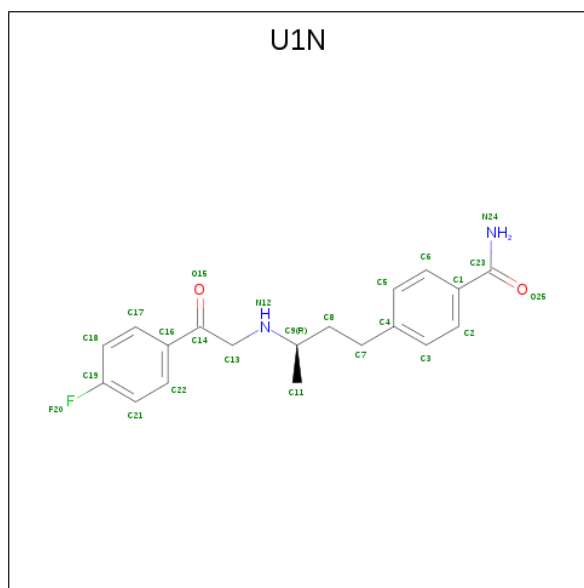
There are 3 unique types of molecules in this entry. The entry contains 12514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Dipeptidyl peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			

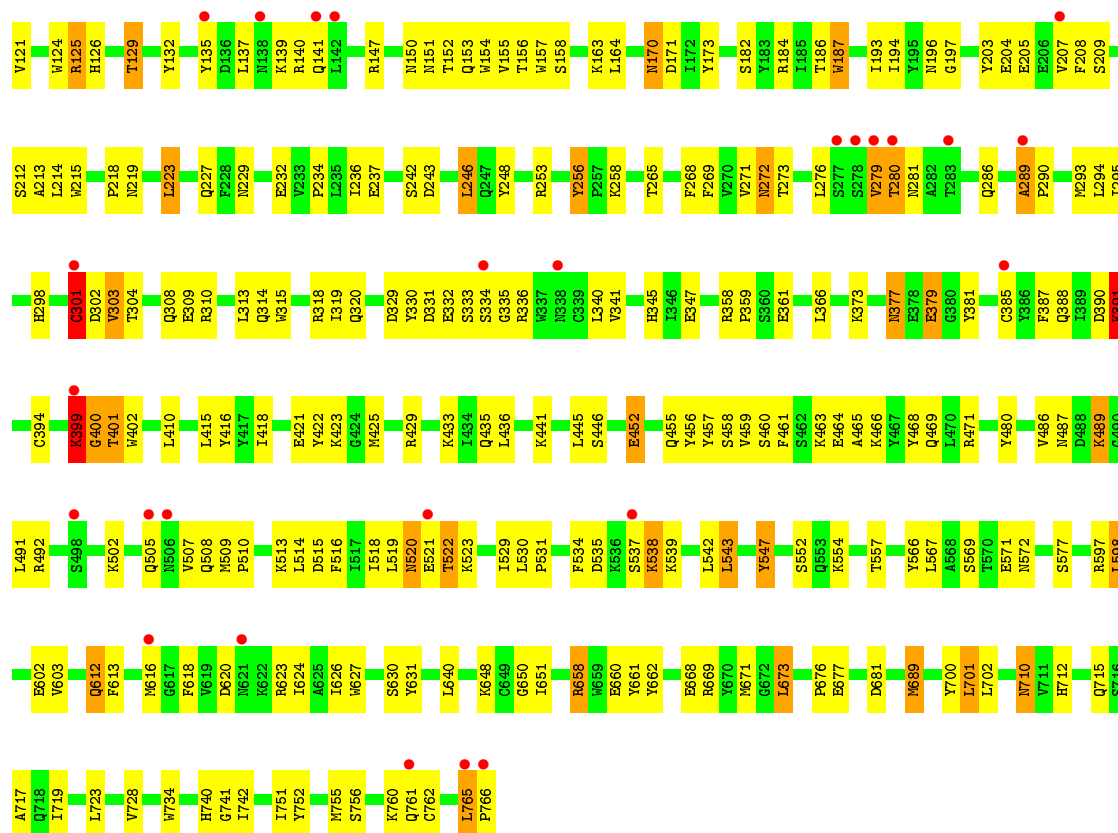
- Molecule 2 is 4-[(3R)-3-{[2-(4-FLUOROPHENYL)-2-OXOETHYL]AMINO}BUTYL]BENZAMIDE (three-letter code: U1N) (formula: C₁₉H₂₁FN₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	19	1	2	2		
2	B	1	Total	C	F	N	O	0	0
			24	19	1	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	269	Total 269	O 269	0	0
3	B	285	Total 285	O 285	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.59Å 122.30Å 112.72Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 45.73 – 2.11	Depositor EDS
% Data completeness (in resolution range)	84.4 (50.00-2.10) 86.2 (45.73-2.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.268 0.224 , 0.260	Depositor DCC
R_{free} test set	4231 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12514	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: U1N

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	0.37	0/6119	0.66	1/8321 (0.0%)
1	B	0.38	1/6136 (0.0%)	0.66	3/8344 (0.0%)
All	All	0.38	1/12255 (0.0%)	0.66	4/16665 (0.0%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	301	CYS	CB-SG	-6.00	1.72	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	LYS	N-CA-C	5.46	125.74	111.00
1	B	319	ILE	N-CA-C	-5.28	96.73	111.00
1	B	400	GLY	N-CA-C	5.24	126.19	113.10
1	A	547	TYR	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	700	TYR	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	A	5948	0	5667	264	0
1	B	5964	0	5685	276	0
2	A	24	0	21	1	0
2	B	24	0	21	1	0
3	A	269	0	0	26	0
3	B	285	0	0	23	0
All	All	12514	0	11394	529	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 23.

All (529) 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)
1:B:651:ILE:HG21	1:B:755:MET:HE3	1.36	1.06
1:A:392:LYS:HD2	1:A:393:ASP:N	1.72	1.05
1:B:69:LEU:HD13	1:B:76:ILE:HD11	1.41	1.02
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.55	1.02
1:A:487:ASN:HB2	1:A:489:LYS:HD2	1.42	0.99
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.42	0.98
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.46	0.97
1:A:392:LYS:HD2	1:A:393:ASP:H	1.35	0.88
1:B:219:ASN:HB2	1:B:308:GLN:CD	1.95	0.88
1:A:172:ILE:H	1:A:186:THR:HG22	1.36	0.87
1:A:177:GLU:HB2	1:A:180:LEU:HD13	1.55	0.87
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.03	0.87
1:A:172:ILE:H	1:A:186:THR:CG2	1.86	0.86
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.05	0.86
1:B:121:VAL:HB	1:B:129:THR:HG23	1.59	0.85
1:B:203:TYR:CD2	1:B:207:VAL:HG21	2.12	0.85
1:A:519:LEU:HG	3:A:1001:HOH:O	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:LYS:HB3	1:B:765:LEU:HD22	1.59	0.84
1:A:580:GLY:O	1:A:583:SER:HB2	1.79	0.82
1:B:756:SER:O	1:B:760:LYS:HG2	1.79	0.82
1:B:93:SER:HB2	1:B:96:ASP:OD2	1.79	0.81
1:A:284:SER:HA	3:A:1023:HOH:O	1.79	0.81
1:A:89:PHE:HD1	1:A:90:LEU:HD12	1.45	0.80
1:A:271:VAL:HB	3:A:1023:HOH:O	1.81	0.80
1:B:399:LYS:HB2	1:B:402:TRP:CZ2	2.16	0.79
1:B:184:ARG:HD3	1:B:186:THR:O	1.81	0.78
1:B:218:PRO:HG2	1:B:308:GLN:OE1	1.84	0.78
1:A:139:LYS:HG3	1:A:141:GLN:HB2	1.66	0.78
1:A:630:SER:HG	1:A:740:HIS:HE2	1.31	0.78
1:A:253:ARG:HH22	1:B:253:ARG:HH21	1.31	0.77
1:A:152:THR:HA	3:A:912:HOH:O	1.82	0.77
1:A:487:ASN:HB2	1:A:489:LYS:CD	2.15	0.77
1:B:279:VAL:HG23	1:B:280:THR:H	1.49	0.77
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.82	0.77
1:B:538:LYS:CE	1:B:539:LYS:H	1.98	0.76
1:B:401:THR:O	1:B:401:THR:HG22	1.85	0.76
1:A:596:ARG:O	1:A:597:ARG:HD2	1.86	0.75
1:A:736:THR:HG21	1:B:717:ALA:O	1.86	0.75
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.85	0.75
1:B:40:ARG:HG2	1:B:508:GLN:HG3	1.70	0.74
1:B:765:LEU:HB3	1:B:766:PRO:CA	2.18	0.74
1:A:407:ILE:HG23	3:A:1002:HOH:O	1.86	0.73
1:A:168:TRP:HB2	3:A:912:HOH:O	1.86	0.73
1:A:114:ILE:CD1	1:A:137:LEU:HD21	2.19	0.72
1:B:471:ARG:NH1	1:B:480:TYR:HE2	1.86	0.72
1:B:336:ARG:HB3	3:B:866:HOH:O	1.89	0.72
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.03	0.72
1:A:341:VAL:O	1:A:342:ALA:HB3	1.90	0.71
1:A:341:VAL:HG12	3:A:996:HOH:O	1.89	0.71
1:A:438:ASP:OD1	1:A:440:THR:HB	1.91	0.71
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	1.39	0.71
1:B:98:PHE:CD1	1:B:100:HIS:HB2	2.26	0.70
1:B:538:LYS:HE3	1:B:539:LYS:H	1.57	0.70
1:A:207:VAL:HG22	1:A:208:PHE:HD1	1.55	0.70
1:B:471:ARG:HH11	1:B:480:TYR:HE2	1.40	0.70
1:A:579:ASP:HB3	1:A:583:SER:OG	1.93	0.69
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.28	0.68
1:B:207:VAL:HG23	1:B:208:PHE:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:765:LEU:HB3	1:B:766:PRO:OXT	1.93	0.68
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.91	0.68
1:B:137:LEU:O	1:B:140:ARG:HD2	1.94	0.67
1:A:207:VAL:HG22	1:A:208:PHE:CD1	2.29	0.67
1:B:280:THR:HG23	1:B:281:ASN:N	2.09	0.67
1:B:61:ARG:HD2	3:B:819:HOH:O	1.93	0.67
1:B:69:LEU:HD13	1:B:76:ILE:CD1	2.21	0.67
1:B:203:TYR:O	1:B:207:VAL:HG22	1.93	0.67
1:B:399:LYS:HB2	1:B:402:TRP:HZ2	1.60	0.67
1:B:308:GLN:OE1	1:B:308:GLN:HA	1.93	0.67
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.60	0.67
1:A:415:LEU:HD13	3:A:1002:HOH:O	1.95	0.67
1:B:203:TYR:HD2	1:B:207:VAL:HG21	1.57	0.67
1:B:630:SER:HG	1:B:740:HIS:HE2	1.41	0.67
1:B:301:CYS:SG	1:B:359:PRO:HD2	2.36	0.66
1:A:463:LYS:HG2	3:A:901:HOH:O	1.93	0.66
1:A:253:ARG:NH2	1:B:253:ARG:NH2	2.39	0.66
1:B:71:LYS:HB2	3:B:787:HOH:O	1.94	0.66
1:B:75:ASN:HB3	1:B:92:ASN:N	2.11	0.66
1:B:310:ARG:HG3	1:B:329:ASP:OD1	1.94	0.66
1:B:289:ALA:HA	1:B:294:LEU:HD11	1.78	0.66
1:B:51:ASN:HD21	1:B:54:ARG:HD3	1.61	0.65
1:B:289:ALA:CB	1:B:290:PRO:HA	2.24	0.65
1:B:377:ASN:C	1:B:377:ASN:HD22	1.99	0.65
1:A:76:ILE:HB	1:A:90:LEU:CD1	2.27	0.65
1:A:370:SER:HB2	1:A:387:PHE:O	1.96	0.64
1:A:310:ARG:HH12	1:A:343:ARG:NH2	1.95	0.64
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.78	0.64
1:B:219:ASN:HB2	1:B:308:GLN:OE1	1.98	0.64
1:A:544:LEU:HD21	1:A:606:GLN:HG3	1.79	0.64
1:B:280:THR:HG23	1:B:281:ASN:H	1.63	0.64
1:A:90:LEU:O	1:A:90:LEU:HD22	1.98	0.63
1:B:40:ARG:HH11	1:B:508:GLN:HG2	1.62	0.63
1:A:392:LYS:CD	1:A:393:ASP:H	2.08	0.63
1:A:71:LYS:NZ	1:A:105:TYR:HB2	2.13	0.63
1:B:651:ILE:HG21	1:B:755:MET:CE	2.22	0.63
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.99	0.63
1:A:522:THR:HG21	1:A:590:ILE:HD11	1.81	0.63
1:B:51:ASN:HD21	1:B:54:ARG:CD	2.12	0.63
1:A:377:ASN:HB3	1:A:379:GLU:H	1.62	0.62
1:B:126:HIS:HE1	3:B:770:HOH:O	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:MET:HE2	1:A:574:ILE:HG21	1.82	0.62
1:B:58:TYR:HD1	1:B:60:LEU:HD11	1.65	0.62
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.00	0.62
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.43	0.62
1:A:314:GLN:HG3	1:A:325:MET:HG3	1.82	0.62
1:B:125:ARG:HG2	1:B:126:HIS:CE1	2.35	0.62
1:A:152:THR:HG21	1:A:155:VAL:CG2	2.29	0.61
1:A:177:GLU:CB	1:A:180:LEU:HD13	2.28	0.61
1:B:126:HIS:HD2	3:B:905:HOH:O	1.83	0.61
1:B:139:LYS:HG3	1:B:141:GLN:HB2	1.81	0.61
1:B:400:GLY:HA2	3:B:1040:HOH:O	2.00	0.61
1:A:452:GLU:HG2	3:A:985:HOH:O	2.01	0.61
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.00	0.61
1:B:289:ALA:HB2	3:B:934:HOH:O	1.99	0.61
1:B:765:LEU:HB3	1:B:766:PRO:HA	1.81	0.61
1:A:289:ALA:CB	1:A:290:PRO:HA	2.25	0.61
1:B:502:LYS:O	1:B:505:GLN:HG2	2.00	0.61
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.36	0.61
1:B:452:GLU:HG3	3:B:1004:HOH:O	2.01	0.60
1:B:205:GLU:OE2	2:B:767:U1N:H111	2.00	0.60
1:B:98:PHE:HD1	1:B:100:HIS:HB2	1.66	0.60
1:A:295:ILE:HD11	1:A:317:ARG:NH2	2.17	0.60
1:A:482:LEU:HD12	3:A:979:HOH:O	2.01	0.60
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.37	0.60
1:A:55:LEU:CD1	1:A:561:LEU:HD22	2.31	0.60
1:B:207:VAL:CG2	1:B:208:PHE:N	2.65	0.60
1:B:765:LEU:CB	1:B:766:PRO:HA	2.31	0.60
1:B:415:LEU:HD23	1:B:415:LEU:C	2.22	0.60
1:B:723:LEU:HB3	1:B:728:VAL:HG13	1.84	0.60
1:B:318:ARG:HD3	1:B:668:GLU:OE1	2.02	0.59
1:B:295:ILE:O	1:B:295:ILE:HG12	2.03	0.59
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.37	0.59
1:A:392:LYS:HE3	1:A:393:ASP:OD2	2.03	0.59
1:A:523:LYS:HD2	3:A:933:HOH:O	2.01	0.59
1:B:471:ARG:NH1	1:B:480:TYR:CE2	2.70	0.59
1:A:372:TYR:OH	1:A:436:LEU:HG	2.01	0.59
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.33	0.59
1:B:170:ASN:N	1:B:170:ASN:HD22	1.99	0.59
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.84	0.59
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.83	0.59
1:A:295:ILE:HD11	1:A:317:ARG:HH21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ARG:HG2	1:A:661:TYR:CD2	2.38	0.59
1:B:302:ASP:OD1	1:B:304:THR:HG23	2.03	0.58
1:B:279:VAL:HG23	1:B:280:THR:N	2.17	0.58
1:B:289:ALA:HA	1:B:294:LEU:CD1	2.33	0.58
1:B:358:ARG:HH11	1:B:358:ARG:HG2	1.68	0.58
1:A:111:GLY:O	1:A:137:LEU:HD12	2.04	0.58
1:B:520:ASN:O	1:B:521:GLU:HB3	2.03	0.58
1:B:289:ALA:CB	1:B:290:PRO:CA	2.78	0.58
1:A:306:ALA:HB3	1:A:310:ARG:HB3	1.86	0.57
1:A:89:PHE:CD1	1:A:90:LEU:HD12	2.33	0.57
1:B:445:LEU:HD22	1:B:445:LEU:N	2.19	0.57
1:B:69:LEU:CD1	1:B:76:ILE:HD11	2.25	0.57
1:B:723:LEU:HD22	1:B:728:VAL:HG11	1.86	0.57
1:A:486:VAL:HG13	1:A:487:ASN:N	2.19	0.57
1:A:581:ARG:HG2	1:A:593:ALA:CB	2.35	0.57
1:A:603:VAL:HG23	1:A:639:VAL:HG22	1.85	0.57
1:B:293:MET:HE3	1:B:315:TRP:O	2.03	0.57
1:B:40:ARG:HG2	1:B:508:GLN:CG	2.34	0.57
1:B:83:TYR:HE1	3:B:1035:HOH:O	1.87	0.57
1:A:47:ASP:HA	1:A:52:THR:HG23	1.85	0.57
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.86	0.57
1:A:517:ILE:HG13	3:A:1001:HOH:O	2.05	0.56
1:A:581:ARG:HB2	1:A:605:ASP:OD2	2.04	0.56
1:B:147:ARG:HB3	1:B:147:ARG:NH1	2.19	0.56
1:B:150:ASN:HA	3:B:937:HOH:O	2.04	0.56
1:A:205:GLU:OE2	2:A:767:U1N:H111	2.05	0.56
1:A:76:ILE:HB	1:A:90:LEU:HD11	1.87	0.56
1:A:116:LEU:O	1:A:132:TYR:HA	2.05	0.56
1:A:143:ILE:HD12	1:A:143:ILE:H	1.71	0.56
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.35	0.56
1:B:60:LEU:HD13	1:B:469:GLN:CD	2.26	0.56
1:A:193:ILE:HG22	1:A:194:ILE:HG13	1.86	0.56
1:A:197:GLY:C	1:A:213:ALA:HB3	2.24	0.56
1:A:223:LEU:HB3	1:A:271:VAL:CG1	2.35	0.56
1:A:543:LEU:HD21	1:A:627:TRP:HD1	1.71	0.56
1:B:673:LEU:HD22	3:B:1010:HOH:O	2.06	0.56
1:B:765:LEU:CB	1:B:766:PRO:CA	2.84	0.56
1:B:458:SER:OG	1:B:471:ARG:HB2	2.05	0.56
1:B:602:GLU:HG3	1:B:603:VAL:N	2.22	0.55
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.41	0.55
1:B:40:ARG:NH1	1:B:508:GLN:HG2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG22	1:A:166:TYR:HB2	1.87	0.55
1:B:293:MET:HE3	1:B:315:TRP:C	2.26	0.55
1:A:289:ALA:CB	1:A:290:PRO:CA	2.79	0.55
1:B:78:VAL:HG12	1:B:87:SER:O	2.05	0.55
1:B:272:ASN:C	1:B:272:ASN:HD22	2.10	0.55
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.06	0.55
1:A:341:VAL:O	1:A:342:ALA:CB	2.54	0.54
1:A:472:CYS:O	1:A:478:PRO:HA	2.07	0.54
1:B:358:ARG:NH1	1:B:358:ARG:HG2	2.21	0.54
1:B:40:ARG:CG	1:B:508:GLN:HG3	2.37	0.54
1:A:39:SER:O	1:A:40:ARG:HB2	2.08	0.54
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.43	0.54
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.43	0.54
1:A:100:HIS:CD2	3:A:917:HOH:O	2.60	0.54
1:B:78:VAL:HG13	1:B:78:VAL:O	2.07	0.54
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.89	0.54
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.43	0.54
1:A:223:LEU:O	1:A:271:VAL:HG12	2.07	0.54
1:A:114:ILE:HG13	1:A:137:LEU:HD11	1.89	0.54
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.91	0.53
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.39	0.53
1:A:492:ARG:HG3	3:A:979:HOH:O	2.08	0.53
1:A:72:GLN:HB2	1:A:75:ASN:O	2.09	0.53
1:A:581:ARG:HG2	1:A:593:ALA:HB1	1.91	0.53
1:B:630:SER:OG	1:B:740:HIS:NE2	2.27	0.53
1:A:40:ARG:HB3	1:A:506:ASN:O	2.07	0.53
1:A:658:ARG:HD3	1:A:660:GLU:HB2	1.91	0.53
1:B:459:VAL:HG22	1:B:460:SER:N	2.23	0.53
1:A:317:ARG:HG2	3:A:954:HOH:O	2.09	0.53
1:A:528:MET:CE	1:A:574:ILE:HG21	2.37	0.53
1:A:269:PHE:CE2	1:A:286:GLN:HB2	2.44	0.53
1:A:143:ILE:HG23	1:A:145:GLU:OE2	2.09	0.53
1:A:603:VAL:HG23	1:A:639:VAL:CG2	2.39	0.53
1:A:203:TYR:HA	1:A:207:VAL:CG1	2.38	0.52
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.44	0.52
1:A:362:PRO:HA	1:A:373:LYS:HB3	1.91	0.52
1:B:309:GLU:HB2	1:B:330:TYR:HB3	1.91	0.52
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.10	0.52
1:A:286:GLN:HG2	1:A:288:THR:HG22	1.91	0.52
1:A:751:ILE:O	1:A:755:MET:HG3	2.08	0.52
1:B:153:GLN:HE22	1:B:170:ASN:HD21	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLN:NE2	1:A:359:PRO:HB2	2.25	0.52
1:A:289:ALA:HA	1:A:294:LEU:HG	1.91	0.52
1:B:60:LEU:CD1	1:B:469:GLN:NE2	2.72	0.52
1:A:341:VAL:C	1:A:343:ARG:H	2.12	0.52
1:A:658:ARG:O	1:A:658:ARG:HG3	2.09	0.52
1:B:415:LEU:HD23	1:B:416:TYR:N	2.25	0.52
1:B:630:SER:HG	1:B:740:HIS:CE1	2.27	0.52
1:B:76:ILE:CG2	1:B:90:LEU:HB2	2.39	0.52
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.45	0.52
1:A:139:LYS:CG	1:A:141:GLN:HB2	2.37	0.52
1:A:96:ASP:C	1:A:98:PHE:H	2.14	0.51
1:B:147:ARG:HH11	1:B:147:ARG:HB3	1.75	0.51
1:B:651:ILE:CG2	1:B:755:MET:HE3	2.25	0.51
1:A:377:ASN:HB2	1:A:381:TYR:O	2.10	0.51
1:B:390:ASP:CG	1:B:390:ASP:O	2.48	0.51
1:B:391:LYS:HD3	3:B:889:HOH:O	2.11	0.51
1:B:332:GLU:HG2	1:B:332:GLU:O	2.11	0.51
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.91	0.51
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.10	0.51
1:B:535:ASP:OD1	1:B:537:SER:HB2	2.11	0.51
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.10	0.51
1:B:401:THR:O	1:B:401:THR:CG2	2.57	0.51
1:B:60:LEU:HD13	1:B:469:GLN:OE1	2.11	0.51
1:A:597:ARG:HH12	1:A:679:ASN:HD21	1.57	0.51
1:B:72:GLN:C	1:B:74:ASN:H	2.15	0.51
1:B:531:PRO:HB3	1:B:572:ASN:HD22	1.75	0.51
1:B:602:GLU:OE1	1:B:631:TYR:HE1	1.94	0.50
1:B:487:ASN:OD1	1:B:489:LYS:HB3	2.11	0.50
1:B:765:LEU:HB3	1:B:766:PRO:C	2.31	0.50
1:A:215:TRP:CZ3	1:A:268:PHE:HE1	2.28	0.50
1:A:273:THR:O	1:A:276:LEU:CD2	2.60	0.50
1:B:289:ALA:HB3	3:B:964:HOH:O	2.11	0.50
1:B:77:LEU:HD22	1:B:88:VAL:HA	1.93	0.50
1:B:98:PHE:CE1	1:B:100:HIS:HB2	2.46	0.50
1:A:141:GLN:HE21	1:A:141:GLN:N	2.10	0.50
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.94	0.50
1:A:741:GLY:O	1:A:742:ILE:C	2.48	0.50
1:B:157:TRP:CZ3	1:B:164:LEU:HG	2.47	0.50
1:B:466:LYS:HD3	3:B:926:HOH:O	2.12	0.50
1:B:387:PHE:CE1	1:B:394:CYS:HB3	2.47	0.50
1:B:598:LEU:HB2	1:B:671:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HD12	1:A:137:LEU:HD21	1.92	0.50
1:A:143:ILE:HD12	1:A:143:ILE:N	2.27	0.50
1:A:392:LYS:CD	1:A:393:ASP:N	2.60	0.50
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.46	0.50
1:B:377:ASN:ND2	1:B:381:TYR:H	2.09	0.50
1:A:546:VAL:CG2	1:A:547:TYR:N	2.74	0.50
1:B:39:SER:O	1:B:40:ARG:HB3	2.12	0.50
1:B:455:GLN:HG2	3:B:935:HOH:O	2.12	0.50
1:B:518:ILE:CD1	1:B:523:LYS:HB3	2.41	0.50
1:B:51:ASN:ND2	1:B:54:ARG:HD3	2.25	0.50
1:A:543:LEU:HD21	1:A:627:TRP:CD1	2.47	0.49
1:B:741:GLY:O	1:B:742:ILE:C	2.50	0.49
1:A:310:ARG:NH1	1:A:329:ASP:OD2	2.45	0.49
1:A:756:SER:O	1:A:760:LYS:HG3	2.13	0.49
1:B:129:THR:OG1	1:B:151:ASN:HA	2.12	0.49
1:B:69:LEU:HB3	1:B:76:ILE:HD11	1.94	0.49
1:A:486:VAL:CG1	1:A:487:ASN:N	2.76	0.49
1:A:500:LEU:HA	1:A:503:MET:CE	2.42	0.49
1:A:78:VAL:HG12	1:A:87:SER:O	2.11	0.49
1:A:95:PHE:CE1	1:A:116:LEU:HD11	2.48	0.49
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.76	0.49
1:B:243:ASP:HB3	3:B:849:HOH:O	2.12	0.49
1:B:80:ASN:OD1	1:B:82:GLU:HB3	2.13	0.49
1:B:529:ILE:HD13	3:B:809:HOH:O	2.13	0.49
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.94	0.49
1:B:58:TYR:HD1	1:B:60:LEU:CD1	2.25	0.49
1:B:51:ASN:ND2	1:B:54:ARG:CD	2.74	0.49
1:A:310:ARG:HG3	1:A:329:ASP:OD1	2.13	0.49
1:A:524:PHE:CZ	3:A:887:HOH:O	2.65	0.49
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.36	0.48
1:A:289:ALA:HB1	1:A:290:PRO:C	2.34	0.48
1:A:502:LYS:O	1:A:505:GLN:HG2	2.13	0.48
1:A:55:LEU:HD11	1:A:561:LEU:HD22	1.95	0.48
1:B:534:PHE:HZ	1:B:618:PHE:CD1	2.31	0.48
1:B:158:SER:OG	1:B:163:LYS:HB2	2.14	0.48
1:B:456:TYR:HB2	1:B:557:THR:OG1	2.14	0.48
1:B:519:LEU:O	1:B:522:THR:HG23	2.14	0.48
1:A:458:SER:HB2	1:A:471:ARG:HH21	1.79	0.48
1:B:154:TRP:NE1	1:B:156:THR:HG23	2.29	0.48
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.49	0.48
1:A:154:TRP:CD1	1:A:214:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.96	0.48
1:B:399:LYS:HD2	1:B:421:GLU:OE2	2.13	0.48
1:A:136:ASP:O	1:A:140:ARG:HA	2.14	0.48
1:A:259:ALA:HB3	1:A:660:GLU:HA	1.95	0.48
1:B:197:GLY:C	1:B:213:ALA:HB3	2.35	0.48
1:B:334:SER:OG	1:B:336:ARG:HG2	2.14	0.48
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.95	0.47
1:A:681:ASP:HB2	3:A:1031:HOH:O	2.13	0.47
1:A:70:TYR:O	1:A:72:GLN:N	2.47	0.47
1:B:109:PRO:HG2	1:B:158:SER:O	2.14	0.47
1:A:108:SER:C	1:A:110:ASP:H	2.16	0.47
1:A:514:LEU:HD22	1:A:525:TRP:HE3	1.80	0.47
1:B:124:TRP:HB2	1:B:204:GLU:OE2	2.14	0.47
1:B:648:LYS:HE2	1:B:762:CYS:O	2.14	0.47
1:B:74:ASN:HB3	1:B:92:ASN:OD1	2.15	0.47
1:A:492:ARG:HG2	1:A:492:ARG:NH1	2.30	0.47
1:A:739:ASP:HB2	3:A:774:HOH:O	2.13	0.47
1:B:280:THR:CG2	1:B:281:ASN:N	2.76	0.47
1:B:318:ARG:HG2	3:B:807:HOH:O	2.14	0.47
1:B:760:LYS:HB2	1:B:765:LEU:HB2	1.96	0.47
1:A:154:TRP:NE1	1:A:214:LEU:HD11	2.30	0.47
1:A:535:ASP:OD1	1:A:537:SER:HB3	2.14	0.47
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.61	0.47
1:B:554:LYS:HB3	1:B:577:SER:HB3	1.97	0.47
1:A:543:LEU:HD12	1:A:567:LEU:HD13	1.96	0.47
1:B:538:LYS:HE3	1:B:538:LYS:HA	1.95	0.47
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.63	0.47
1:A:176:ILE:HD12	1:A:176:ILE:N	2.30	0.46
1:A:272:ASN:C	1:A:272:ASN:HD22	2.19	0.46
1:A:415:LEU:HB3	1:A:434:ILE:CG2	2.45	0.46
1:B:377:ASN:ND2	1:B:379:GLU:H	2.12	0.46
1:A:127:SER:O	1:A:128:TYR:HB3	2.16	0.46
1:B:331:ASP:O	1:B:335:GLY:N	2.47	0.46
1:B:345:HIS:HD2	3:B:888:HOH:O	1.99	0.46
1:A:89:PHE:CE1	1:A:107:ILE:HD13	2.51	0.46
1:A:176:ILE:HD13	1:A:183:TYR:CE2	2.50	0.46
1:B:173:TYR:CZ	1:B:184:ARG:HG3	2.51	0.46
1:B:81:ALA:O	1:B:492:ARG:NH2	2.36	0.46
1:B:293:MET:HG3	1:B:298:HIS:CB	2.46	0.46
1:B:377:ASN:HD21	1:B:381:TYR:H	1.64	0.46
1:B:40:ARG:HH11	1:B:40:ARG:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ASP:OD1	1:A:391:LYS:HD3	2.16	0.46
1:A:93:SER:HA	1:A:96:ASP:OD1	2.16	0.46
1:B:58:TYR:CD1	1:B:60:LEU:HD11	2.46	0.46
1:A:341:VAL:HG22	1:A:342:ALA:N	2.30	0.46
1:B:435:GLN:HB2	1:B:441:LYS:HB2	1.98	0.45
1:B:223:LEU:HB3	1:B:271:VAL:HG12	1.99	0.45
1:B:543:LEU:HD12	1:B:567:LEU:HD13	1.99	0.45
1:B:571:GLU:HB3	1:B:765:LEU:HD21	1.98	0.45
1:A:600:THR:O	1:A:603:VAL:HG13	2.17	0.45
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.15	0.45
1:B:280:THR:CG2	1:B:281:ASN:H	2.26	0.45
1:A:114:ILE:HD11	1:A:137:LEU:HD21	1.94	0.45
1:A:143:ILE:CD1	1:A:143:ILE:H	2.29	0.45
1:A:514:LEU:HD22	1:A:525:TRP:CE3	2.51	0.45
1:A:114:ILE:CG1	1:A:137:LEU:HD11	2.45	0.45
1:A:492:ARG:CG	3:A:979:HOH:O	2.64	0.45
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.16	0.45
1:B:64:SER:C	1:B:463:LYS:HB2	2.36	0.45
1:A:142:LEU:O	1:A:144:THR:HG23	2.16	0.45
1:A:290:PRO:HG3	1:A:326:ASP:OD2	2.17	0.45
1:A:528:MET:HE2	1:A:574:ILE:CG2	2.43	0.45
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.90	0.45
1:A:734:TRP:CD1	1:A:736:THR:HG22	2.52	0.45
1:B:104:ASP:OD1	1:B:105:TYR:N	2.45	0.45
1:A:217:SER:HB3	1:A:222:PHE:HB2	1.99	0.45
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.99	0.45
1:A:76:ILE:HB	1:A:90:LEU:HD13	1.98	0.45
1:B:268:PHE:CD2	1:B:313:LEU:HD21	2.52	0.45
1:B:751:ILE:O	1:B:755:MET:HG3	2.16	0.45
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.52	0.45
1:A:242:SER:OG	1:A:243:ASP:N	2.48	0.45
1:B:258:LYS:NZ	1:B:712:HIS:CD2	2.78	0.45
1:A:77:LEU:CD2	1:A:88:VAL:HG22	2.47	0.44
1:A:105:TYR:N	1:A:105:TYR:CD1	2.85	0.44
1:A:154:TRP:HE1	1:A:214:LEU:HD11	1.82	0.44
1:B:289:ALA:HB1	1:B:290:PRO:C	2.38	0.44
1:A:248:TYR:CE2	1:B:234:PRO:HB2	2.52	0.44
1:B:509:MET:HG3	1:B:510:PRO:HD2	1.99	0.44
1:B:547:TYR:C	1:B:547:TYR:CD2	2.91	0.44
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.52	0.44
1:A:340:LEU:HD12	1:A:343:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ARG:HH11	1:A:492:ARG:HG2	1.82	0.44
1:B:538:LYS:HD3	1:B:539:LYS:N	2.32	0.44
1:B:289:ALA:CA	1:B:294:LEU:HD11	2.47	0.44
1:B:214:LEU:HD12	1:B:214:LEU:O	2.17	0.44
1:B:281:ASN:ND2	3:B:792:HOH:O	2.50	0.44
1:A:145:GLU:CG	1:A:179:ASN:HB2	2.48	0.44
1:A:60:LEU:HD12	1:A:60:LEU:O	2.17	0.44
1:B:273:THR:HA	1:B:276:LEU:HG	2.00	0.44
1:B:60:LEU:HD11	1:B:469:GLN:NE2	2.32	0.44
1:A:542:LEU:HD23	1:A:542:LEU:C	2.39	0.43
1:B:418:ILE:CG2	1:B:429:ARG:HG3	2.48	0.43
1:B:547:TYR:CD1	1:B:552:SER:HB2	2.53	0.43
1:B:658:ARG:HG3	1:B:658:ARG:O	2.17	0.43
1:B:662:TYR:OH	1:B:710:ASN:ND2	2.47	0.43
1:A:133:ASP:OD1	1:A:147:ARG:NH2	2.51	0.43
1:A:432:TYR:CE2	1:A:444:CYS:HB2	2.52	0.43
1:A:547:TYR:CD1	1:A:547:TYR:C	2.91	0.43
1:A:60:LEU:HD12	1:A:60:LEU:C	2.38	0.43
1:B:715:GLN:O	1:B:719:ILE:HG13	2.18	0.43
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.29	0.43
1:A:280:THR:HG22	1:A:281:ASN:N	2.34	0.43
1:B:489:LYS:O	1:B:489:LYS:HG3	2.17	0.43
1:A:295:ILE:CD1	1:A:317:ARG:HH21	2.31	0.43
1:A:612:GLN:HB3	1:A:612:GLN:HE21	1.53	0.43
1:A:63:ILE:CG2	1:A:69:LEU:HG	2.49	0.43
1:B:385:CYS:SG	1:B:387:PHE:CE2	3.11	0.43
1:B:377:ASN:C	1:B:377:ASN:ND2	2.69	0.43
1:B:613:PHE:O	1:B:616:MET:HB2	2.19	0.43
1:A:145:GLU:OE2	1:A:179:ASN:HB2	2.19	0.43
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.18	0.43
1:A:519:LEU:O	1:A:520:ASN:C	2.57	0.43
1:B:242:SER:CB	1:B:246:LEU:HD12	2.48	0.43
1:B:237:GLU:HG2	1:B:253:ARG:HG2	2.00	0.43
1:B:446:SER:HB2	1:B:457:TYR:CE2	2.54	0.43
1:A:254:VAL:HA	1:A:255:PRO:HD3	1.91	0.43
1:B:152:THR:HG21	1:B:155:VAL:HG22	2.00	0.43
1:B:51:ASN:HD21	1:B:54:ARG:HG3	1.83	0.43
1:A:273:THR:HA	1:A:276:LEU:HD22	2.01	0.43
1:A:41:LYS:O	1:A:508:GLN:N	2.44	0.43
1:A:458:SER:OG	1:A:471:ARG:HB2	2.19	0.43
1:A:489:LYS:NZ	3:A:1013:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:VAL:HG22	1:A:547:TYR:N	2.34	0.43
1:B:515:ASP:CG	1:B:516:PHE:H	2.22	0.43
1:B:74:ASN:O	1:B:92:ASN:HA	2.18	0.43
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.94	0.43
1:B:51:ASN:HD21	1:B:54:ARG:CG	2.32	0.43
1:A:325:MET:CE	1:A:327:ILE:HD11	2.49	0.42
1:A:626:ILE:O	1:A:650:GLY:HA2	2.18	0.42
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.39	0.42
1:B:723:LEU:CD2	1:B:728:VAL:HG11	2.48	0.42
1:A:171:ASP:OD1	1:A:186:THR:HG23	2.19	0.42
1:A:568:ALA:HA	1:A:573:ILE:O	2.19	0.42
1:B:723:LEU:O	1:B:728:VAL:HG12	2.19	0.42
1:A:115:LEU:HD21	1:A:155:VAL:HG11	2.01	0.42
1:A:247:GLN:HG2	1:B:258:LYS:HD2	2.02	0.42
1:B:347:GLU:OE1	1:B:373:LYS:NZ	2.48	0.42
1:B:571:GLU:OE1	1:B:765:LEU:HD23	2.19	0.42
1:B:648:LYS:HD3	1:B:762:CYS:SG	2.59	0.42
1:B:208:PHE:O	1:B:209:SER:C	2.57	0.42
1:B:269:PHE:CE2	1:B:286:GLN:HG3	2.54	0.42
1:B:215:TRP:CZ2	1:B:303:VAL:HG11	2.54	0.42
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.02	0.42
1:A:172:ILE:N	1:A:186:THR:HG22	2.19	0.42
1:A:319:ILE:C	1:A:321:ASN:H	2.22	0.42
1:A:415:LEU:C	1:A:415:LEU:CD1	2.87	0.42
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.55	0.42
1:B:491:LEU:O	1:B:492:ARG:HB3	2.19	0.42
1:B:518:ILE:HD11	1:B:523:LYS:HB3	2.01	0.42
1:B:734:TRP:CD1	1:B:734:TRP:C	2.93	0.42
1:A:607:ILE:HG22	1:A:611:ARG:NH1	2.34	0.42
1:A:62:TRP:HB3	3:A:901:HOH:O	2.18	0.42
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.55	0.42
1:B:518:ILE:HD13	1:B:523:LYS:HA	2.02	0.42
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.19	0.42
1:A:134:ILE:O	1:A:143:ILE:HD13	2.19	0.42
1:A:344:GLN:HE21	1:A:346:ILE:HD11	1.85	0.42
1:A:503:MET:O	1:A:506:ASN:HB3	2.19	0.42
1:A:657:SER:HB2	1:A:689:MET:SD	2.60	0.42
1:B:651:ILE:HG23	1:B:701:LEU:HB3	2.02	0.42
1:A:691:ARG:HG3	1:A:691:ARG:HH11	1.85	0.42
1:B:116:LEU:O	1:B:132:TYR:HA	2.20	0.42
1:B:612:GLN:HE21	1:B:612:GLN:HB3	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:HB3	1:A:163:LYS:HB2	2.02	0.42
1:B:171:ASP:OD1	1:B:184:ARG:NH1	2.53	0.42
1:B:518:ILE:HD13	1:B:523:LYS:CA	2.49	0.42
1:A:518:ILE:C	3:A:1001:HOH:O	2.58	0.41
1:A:96:ASP:O	1:A:98:PHE:N	2.53	0.41
1:B:86:SER:O	1:B:87:SER:HB3	2.20	0.41
1:A:327:ILE:HD12	1:A:343:ARG:O	2.21	0.41
1:B:61:ARG:HH12	1:B:107:ILE:H	1.67	0.41
1:B:215:TRP:CE2	1:B:303:VAL:CG1	3.03	0.41
1:B:529:ILE:HD11	3:B:848:HOH:O	2.20	0.41
1:A:177:GLU:HB2	1:A:180:LEU:CD1	2.39	0.41
1:A:463:LYS:NZ	3:A:901:HOH:O	2.54	0.41
1:A:47:ASP:HA	1:A:52:THR:CG2	2.49	0.41
1:A:500:LEU:HA	1:A:503:MET:HE3	2.02	0.41
1:A:736:THR:HG23	3:B:793:HOH:O	2.19	0.41
1:B:75:ASN:HD22	1:B:92:ASN:HB2	1.85	0.41
1:A:531:PRO:HA	1:A:532:PRO:HD3	1.90	0.41
1:B:658:ARG:HD3	1:B:660:GLU:HB2	2.01	0.41
1:A:41:LYS:NZ	1:A:47:ASP:OD2	2.52	0.41
1:A:718:GLN:NE2	1:A:718:GLN:HA	2.36	0.41
1:B:215:TRP:CE2	1:B:303:VAL:HG11	2.55	0.41
1:A:596:ARG:C	1:A:597:ARG:HD2	2.38	0.41
1:B:114:ILE:HG22	1:B:135:TYR:HB3	2.01	0.41
1:A:253:ARG:HH21	1:B:253:ARG:NH2	2.10	0.41
1:A:726:VAL:HG12	1:A:728:VAL:HG23	2.03	0.41
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.20	0.41
1:A:543:LEU:HD23	1:A:544:LEU:N	2.36	0.41
1:A:726:VAL:O	1:A:726:VAL:HG13	2.21	0.41
1:B:518:ILE:HD13	1:B:523:LYS:HB3	2.02	0.41
1:B:571:GLU:HB3	1:B:765:LEU:CD2	2.51	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.41
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.56	0.41
1:A:513:LYS:HE3	1:A:530:LEU:HD11	2.03	0.41
1:B:154:TRP:CE2	1:B:156:THR:HG23	2.56	0.41
1:B:256:TYR:CD1	1:B:256:TYR:C	2.94	0.41
1:B:433:LYS:HB3	1:B:445:LEU:HD21	2.02	0.41
1:B:538:LYS:HE3	1:B:539:LYS:N	2.32	0.41
1:B:69:LEU:HA	1:B:77:LEU:O	2.21	0.41
1:B:751:ILE:HG23	1:B:752:TYR:N	2.35	0.41
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.02	0.40
1:B:464:GLU:O	1:B:465:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD12	1:B:60:LEU:N	2.36	0.40
1:A:139:LYS:CD	1:A:141:GLN:HB2	2.52	0.40
1:A:236:ILE:HG22	1:A:254:VAL:O	2.22	0.40
1:B:137:LEU:O	1:B:140:ARG:CD	2.67	0.40
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.56	0.40
1:A:342:ALA:HA	3:A:873:HOH:O	2.21	0.40
1:A:310:ARG:NH1	1:A:343:ARG:NH2	2.64	0.40
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.56	0.40
1:A:507:VAL:CG2	1:A:509:MET:HG2	2.52	0.40
1:B:207:VAL:CG2	1:B:208:PHE:H	2.33	0.40
1:B:542:LEU:O	1:B:624:ILE:HA	2.21	0.40
1:B:681:ASP:HB2	3:B:1032:HOH:O	2.22	0.40
1:A:118:TYR:O	1:A:130:ALA:HB1	2.22	0.40
1:A:244:GLU:CD	1:B:689:MET:HG3	2.42	0.40
1:A:415:LEU:HB2	1:A:436:LEU:HD11	2.03	0.40
1:A:718:GLN:NE2	3:A:995:HOH:O	2.55	0.40
1:A:139:LYS:HG3	1:A:141:GLN:H	1.86	0.40
1:A:392:LYS:HD2	1:A:393:ASP:CA	2.48	0.40
1:A:720:SER:O	1:A:724:VAL:HG23	2.21	0.40
1:B:39:SER:O	1:B:40:ARG:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	724/728 (100%)	661 (91%)	55 (8%)	8 (1%)	14	9
1	B	726/728 (100%)	662 (91%)	56 (8%)	8 (1%)	14	9
All	All	1450/1456 (100%)	1323 (91%)	111 (8%)	16 (1%)	14	9

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	289	ALA
1	B	399	LYS
1	B	765	LEU
1	A	71	LYS
1	A	72	GLN
1	A	82	GLU
1	A	97	GLU
1	A	289	ALA
1	A	320	GLN
1	B	280	THR
1	B	391	LYS
1	B	401	THR
1	A	334	SER
1	B	73	GLU
1	A	94	THR
1	B	279	VAL

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	651/653 (100%)	600 (92%)	51 (8%)	12	9
1	B	653/653 (100%)	605 (93%)	48 (7%)	13	10
All	All	1304/1306 (100%)	1205 (92%)	99 (8%)	13	10

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	61	ARG
1	A	90	LEU
1	A	105	TYR
1	A	110	ASP
1	A	141	GLN
1	A	145	GLU
1	A	147	ARG

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	184	ARG
1	A	207	VAL
1	A	214	LEU
1	A	230	ASP
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	256	TYR
1	A	272	ASN
1	A	303	VAL
1	A	313	LEU
1	A	329	ASP
1	A	379	GLU
1	A	385	CYS
1	A	392	LYS
1	A	413	ASP
1	A	415	LEU
1	A	436	LEU
1	A	440	THR
1	A	448	GLU
1	A	472	CYS
1	A	482	LEU
1	A	507	VAL
1	A	514	LEU
1	A	543	LEU
1	A	547	TYR
1	A	561	LEU
1	A	566	TYR
1	A	581	ARG
1	A	597	ARG
1	A	603	VAL
1	A	612	GLN
1	A	630	SER
1	A	655	PRO
1	A	658	ARG
1	A	673	LEU
1	A	679	ASN
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	736	THR

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Mol	Chain	Res	Type
1	A	761	GLN
1	B	54	ARG
1	B	90	LEU
1	B	125	ARG
1	B	129	THR
1	B	170	ASN
1	B	182	SER
1	B	187	TRP
1	B	223	LEU
1	B	232	GLU
1	B	246	LEU
1	B	256	TYR
1	B	272	ASN
1	B	301	CYS
1	B	303	VAL
1	B	333	SER
1	B	340	LEU
1	B	341	VAL
1	B	361	GLU
1	B	366	LEU
1	B	377	ASN
1	B	379	GLU
1	B	388	GLN
1	B	391	LYS
1	B	410	LEU
1	B	425	MET
1	B	436	LEU
1	B	452	GLU
1	B	486	VAL
1	B	489	LYS
1	B	507	VAL
1	B	513	LYS
1	B	514	LEU
1	B	520	ASN
1	B	522	THR
1	B	538	LYS
1	B	543	LEU
1	B	547	TYR
1	B	566	TYR
1	B	597	ARG
1	B	598	LEU
1	B	612	GLN

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Mol	Chain	Res	Type
1	B	658	ARG
1	B	673	LEU
1	B	689	MET
1	B	701	LEU
1	B	702	LEU
1	B	710	ASN
1	B	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	119	ASN
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	338	ASN
1	A	344	GLN
1	A	369	ASN
1	A	483	HIS
1	A	487	ASN
1	A	505	GLN
1	A	572	ASN
1	A	586	GLN
1	A	595	ASN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	697	GLN
1	A	704	HIS
1	A	718	GLN
1	A	731	GLN
1	A	761	GLN
1	B	51	ASN
1	B	75	ASN
1	B	112	GLN
1	B	126	HIS
1	B	138	ASN
1	B	169	ASN

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	281	ASN
1	B	314	GLN
1	B	345	HIS
1	B	377	ASN
1	B	572	ASN
1	B	612	GLN
1	B	679	ASN
1	B	685	ASN
1	B	710	ASN
1	B	712	HIS
1	B	718	GLN
1	B	731	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	U1N	A	767	-	24,25,25	2.05	10 (41%)	30,33,33	1.55	5 (16%)
2	U1N	B	767	-	24,25,25	2.12	10 (41%)	30,33,33	1.52	5 (16%)

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	U1N	A	767	-	-	5/18/18/18	0/2/2/2
2	U1N	B	767	-	-	3/18/18/18	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	767	U1N	C23-N24	5.29	1.43	1.33
2	A	767	U1N	C23-N24	4.97	1.42	1.33
2	B	767	U1N	C22-C16	3.02	1.44	1.39
2	B	767	U1N	C17-C16	2.82	1.44	1.39
2	A	767	U1N	C17-C16	2.77	1.44	1.39
2	B	767	U1N	C6-C1	2.74	1.44	1.39
2	A	767	U1N	C2-C1	2.68	1.43	1.39
2	A	767	U1N	C22-C16	2.64	1.43	1.39
2	B	767	U1N	C18-C17	2.53	1.43	1.38
2	B	767	U1N	C21-C19	2.52	1.42	1.37
2	A	767	U1N	C16-C14	2.49	1.53	1.49
2	A	767	U1N	C21-C19	2.42	1.41	1.37
2	A	767	U1N	C6-C1	2.42	1.43	1.39
2	A	767	U1N	C18-C19	2.37	1.41	1.37
2	B	767	U1N	C1-C23	-2.35	1.47	1.50
2	B	767	U1N	C18-C19	2.31	1.41	1.37
2	B	767	U1N	C2-C1	2.24	1.43	1.39
2	A	767	U1N	C3-C2	2.20	1.42	1.38
2	A	767	U1N	C3-C4	2.10	1.43	1.38
2	B	767	U1N	C6-C5	2.00	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	767	U1N	O25-C23-N24	-4.88	115.65	122.58
2	B	767	U1N	O25-C23-N24	-4.71	115.88	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	767	U1N	O25-C23-C1	3.07	123.30	119.63
2	A	767	U1N	O25-C23-C1	3.01	123.24	119.63
2	A	767	U1N	O15-C14-C16	-2.92	116.61	120.74
2	A	767	U1N	C1-C23-N24	2.80	121.11	117.75
2	B	767	U1N	O15-C14-C16	-2.74	116.86	120.74
2	B	767	U1N	C1-C23-N24	2.55	120.81	117.75
2	B	767	U1N	C11-C9-C8	-2.55	106.64	111.47
2	A	767	U1N	C11-C9-C8	-2.41	106.91	111.47

There are no chirality outliers.

All (8) torsion outliers are listed below:

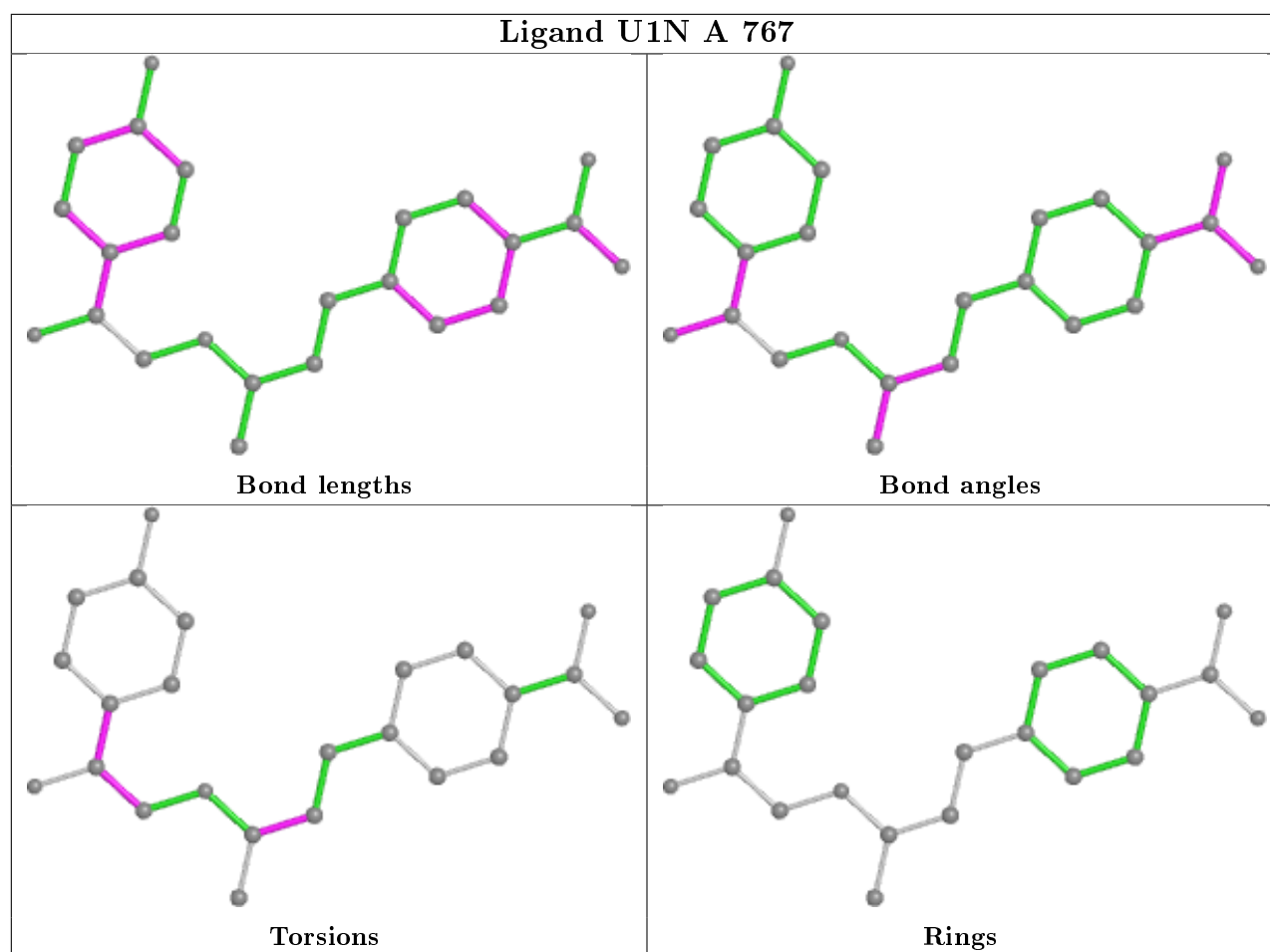
Mol	Chain	Res	Type	Atoms
2	A	767	U1N	C7-C8-C9-C11
2	A	767	U1N	C7-C8-C9-N12
2	A	767	U1N	N12-C13-C14-O15
2	B	767	U1N	N12-C13-C14-O15
2	B	767	U1N	C7-C8-C9-N12
2	A	767	U1N	N12-C13-C14-C16
2	B	767	U1N	N12-C13-C14-C16
2	A	767	U1N	C13-C14-C16-C22

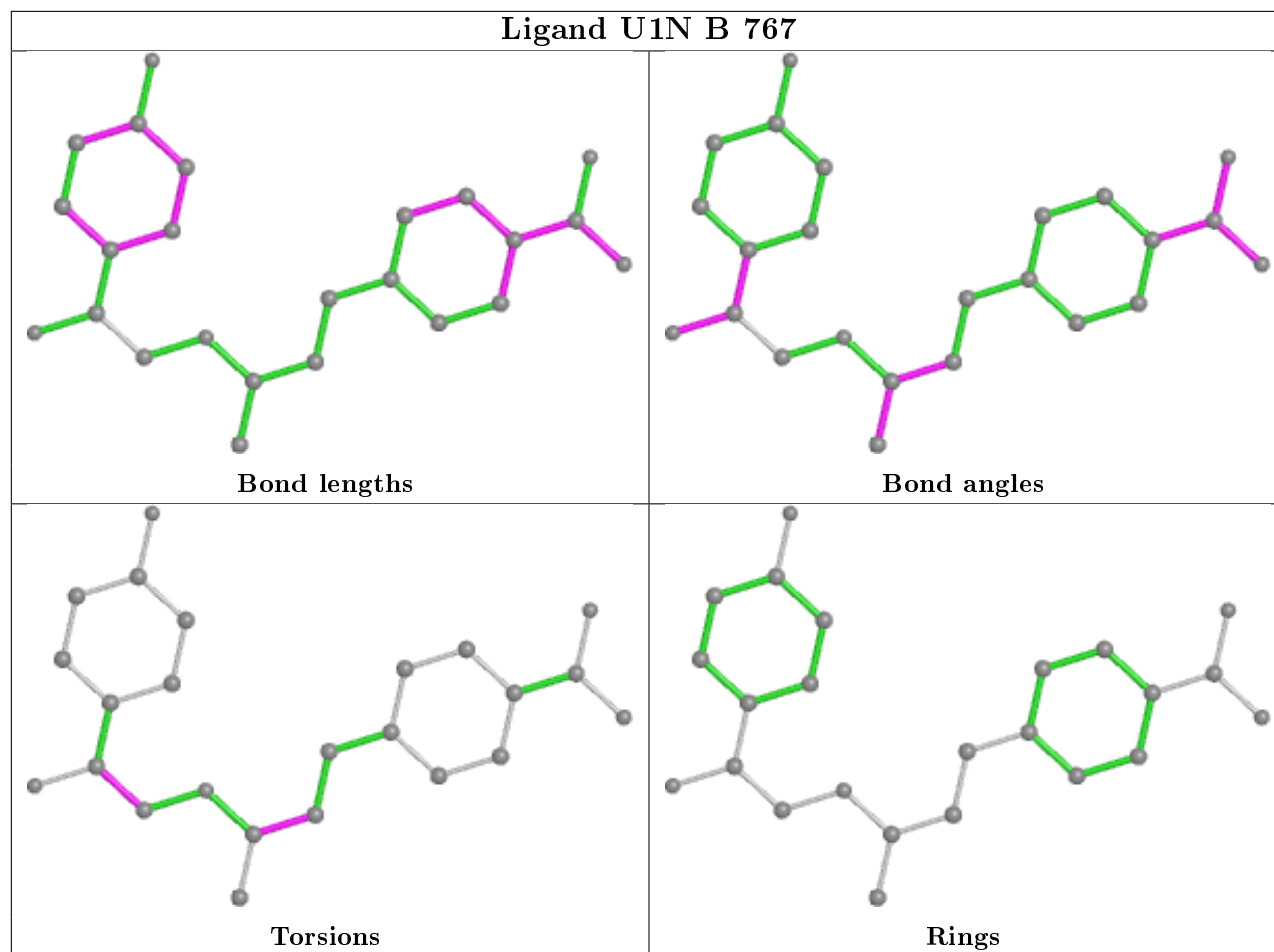
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	767	U1N	1	0
2	B	767	U1N	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	726/728 (99%)	0.46	66 (9%) 9 12	17, 31, 70, 93	0
1	B	728/728 (100%)	0.50	53 (7%) 15 19	18, 31, 62, 87	0
All	All	1454/1456 (99%)	0.48	119 (8%) 11 15	17, 31, 66, 93	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	18.8
1	A	39	SER	11.1
1	B	73	GLU	10.1
1	B	278	SER	9.1
1	B	40	ARG	8.7
1	A	73	GLU	8.1
1	B	97	GLU	8.0
1	B	74	ASN	7.0
1	B	39	SER	6.7
1	A	83	TYR	6.6
1	A	98	PHE	6.1
1	B	277	SER	5.9
1	A	74	ASN	5.8
1	A	90	LEU	5.8
1	A	102	ILE	5.7
1	A	71	LYS	5.7
1	A	84	GLY	5.6
1	A	99	GLY	5.5
1	B	83	TYR	5.5
1	A	105	TYR	5.4
1	A	95	PHE	5.3
1	A	76	ILE	5.3
1	B	766	PRO	5.2
1	A	94	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	139	LYS	4.9
1	A	100	HIS	4.9
1	A	96	ASP	4.6
1	A	101	SER	4.5
1	B	91	GLU	4.5
1	B	72	GLN	4.4
1	B	82	GLU	4.3
1	A	93	SER	4.3
1	B	96	ASP	4.3
1	A	138	ASN	4.2
1	A	135	TYR	4.2
1	B	138	ASN	4.1
1	A	141	GLN	4.1
1	B	92	ASN	4.0
1	B	765	LEU	4.0
1	A	88	VAL	4.0
1	B	99	GLY	3.9
1	B	280	THR	3.8
1	A	103	ASN	3.8
1	B	521	GLU	3.7
1	A	87	SER	3.7
1	A	333	SER	3.7
1	B	81	ALA	3.7
1	A	134	ILE	3.7
1	B	86	SER	3.7
1	A	92	ASN	3.6
1	A	137	LEU	3.5
1	A	91	GLU	3.4
1	A	89	PHE	3.4
1	A	160	VAL	3.4
1	B	71	LYS	3.4
1	A	77	LEU	3.4
1	B	537	SER	3.3
1	B	616	MET	3.2
1	B	87	SER	3.1
1	B	93	SER	3.1
1	A	70	TYR	3.0
1	A	82	GLU	3.0
1	A	148	ILE	2.9
1	B	78	VAL	2.9
1	A	81	ALA	2.9
1	B	385	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	40	ARG	2.8
1	A	97	GLU	2.8
1	B	334	SER	2.8
1	B	505	GLN	2.8
1	A	279	VAL	2.8
1	B	70	TYR	2.8
1	B	338	ASN	2.7
1	B	289	ALA	2.7
1	B	283	THR	2.7
1	A	332	GLU	2.7
1	A	336	ARG	2.7
1	B	301	CYS	2.6
1	A	75	ASN	2.6
1	A	78	VAL	2.6
1	B	141	GLN	2.6
1	B	399	LYS	2.6
1	A	142	LEU	2.5
1	A	86	SER	2.5
1	B	101	SER	2.5
1	A	85	ASN	2.5
1	A	114	ILE	2.5
1	A	289	ALA	2.5
1	A	61	ARG	2.4
1	B	98	PHE	2.4
1	B	88	VAL	2.4
1	B	84	GLY	2.3
1	A	342	ALA	2.3
1	B	621	ASN	2.3
1	A	107	ILE	2.3
1	B	76	ILE	2.3
1	A	110	ASP	2.3
1	B	207	VAL	2.3
1	A	392	LYS	2.3
1	A	492	ARG	2.3
1	A	179	ASN	2.3
1	B	506	ASN	2.3
1	A	69	LEU	2.2
1	A	145	GLU	2.2
1	A	136	ASP	2.2
1	B	761	GLN	2.2
1	A	505	GLN	2.2
1	A	330	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	89	PHE	2.2
1	A	140	ARG	2.1
1	B	135	TYR	2.1
1	B	142	LEU	2.1
1	A	278	SER	2.1
1	A	79	PHE	2.1
1	B	75	ASN	2.1
1	A	536	LYS	2.1
1	B	94	THR	2.0
1	A	335	GLY	2.0
1	B	498	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

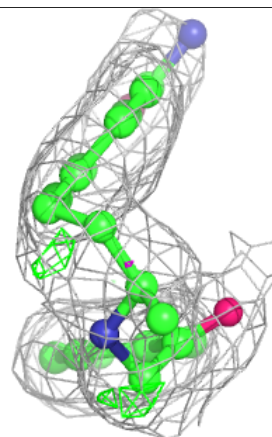
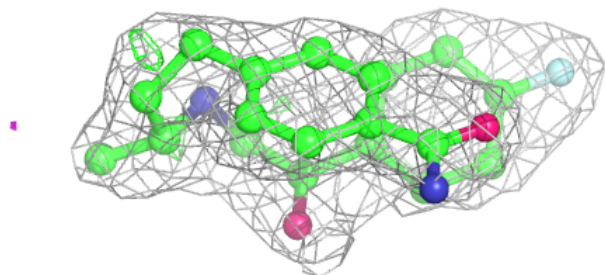
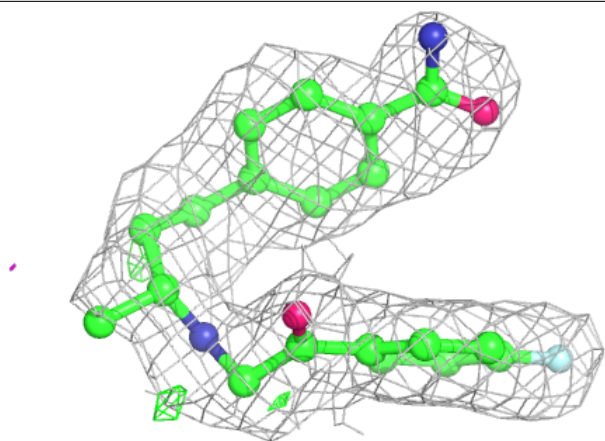
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

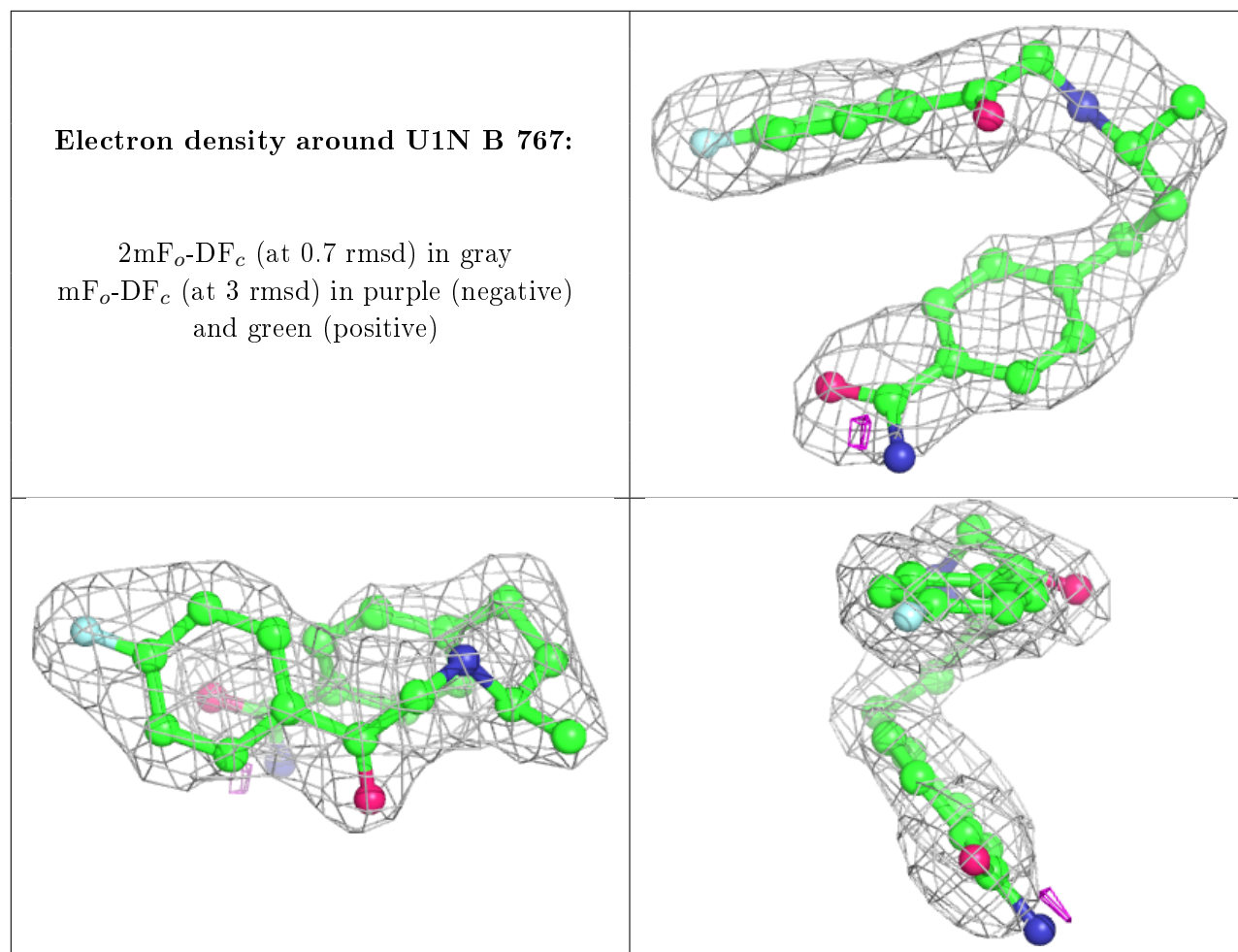
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	U1N	A	767	24/24	0.87	0.22	36,46,50,53	0
2	U1N	B	767	24/24	0.89	0.29	32,48,56,56	0

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

Electron density around U1N A 767:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.