Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:51 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

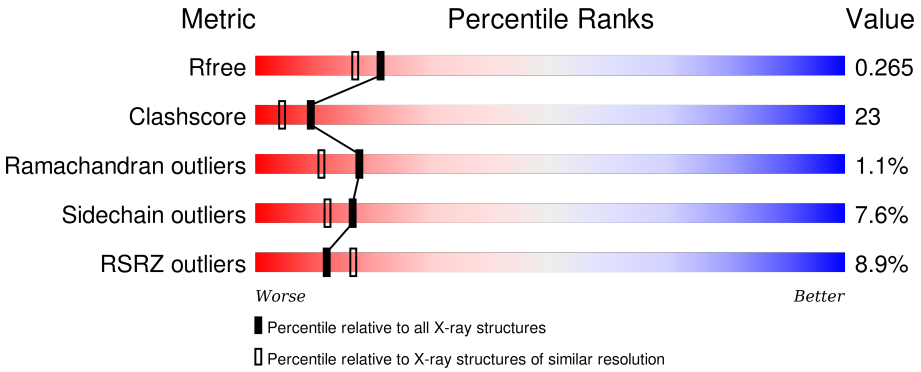
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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 <=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	9% 61% 34% 5%
1	B	728	8% 61% 34% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	U1N	A	767	-	-	-	X
2	U1N	B	767	-	-	-	X

2 Entry composition

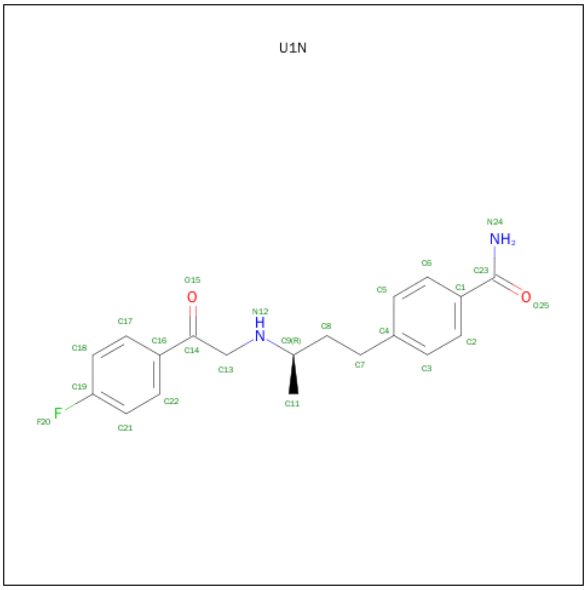
There are 3 unique types of molecules in this entry. The entry contains 12514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_{19}H_{21}FN_2O_2$).



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.

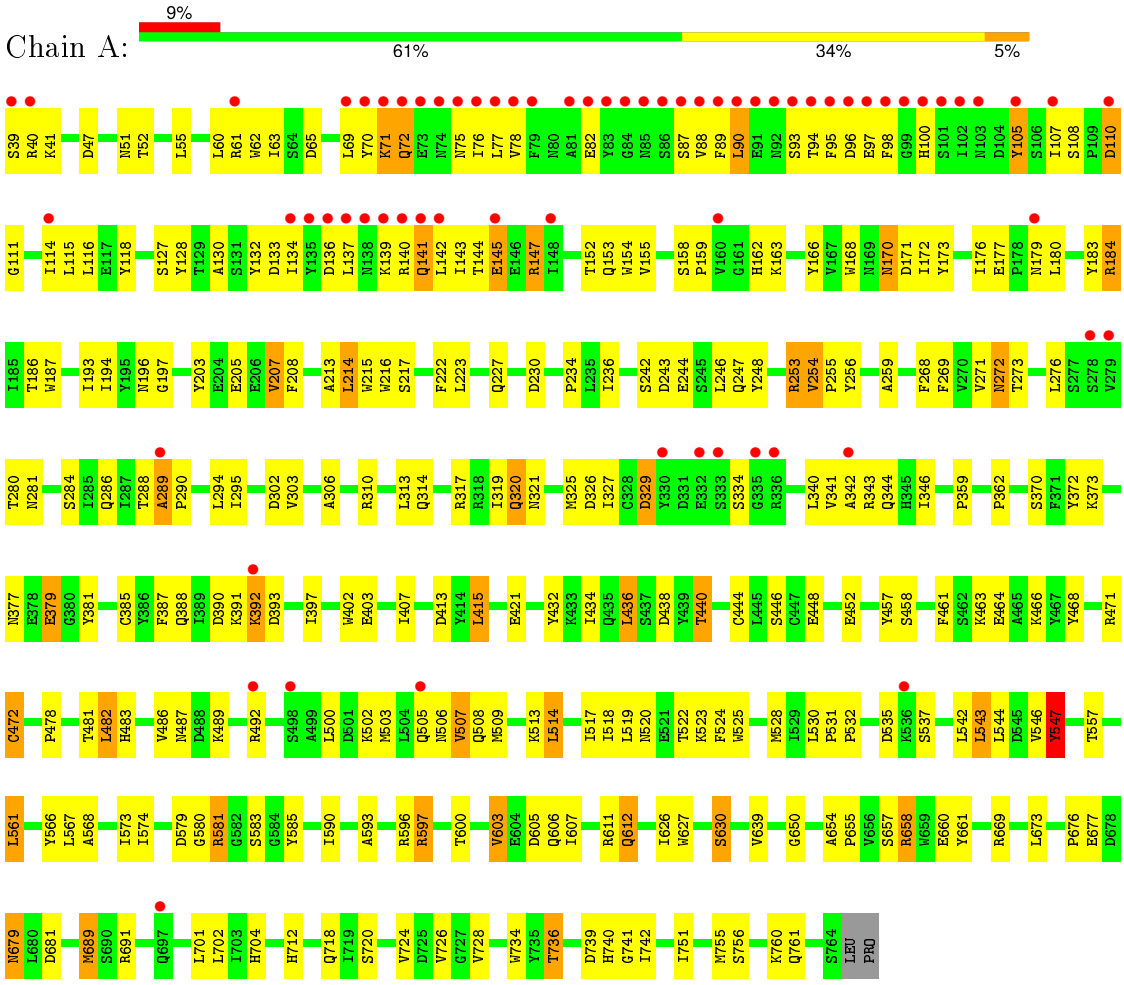
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	269	Total O 269 269	0	0
3	B	285	Total O 285 285	0	0

3 Residue-property plots (i)

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.

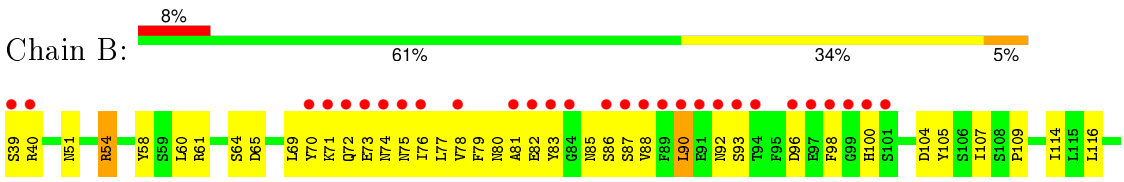
- Molecule 1: Dipeptidyl peptidase

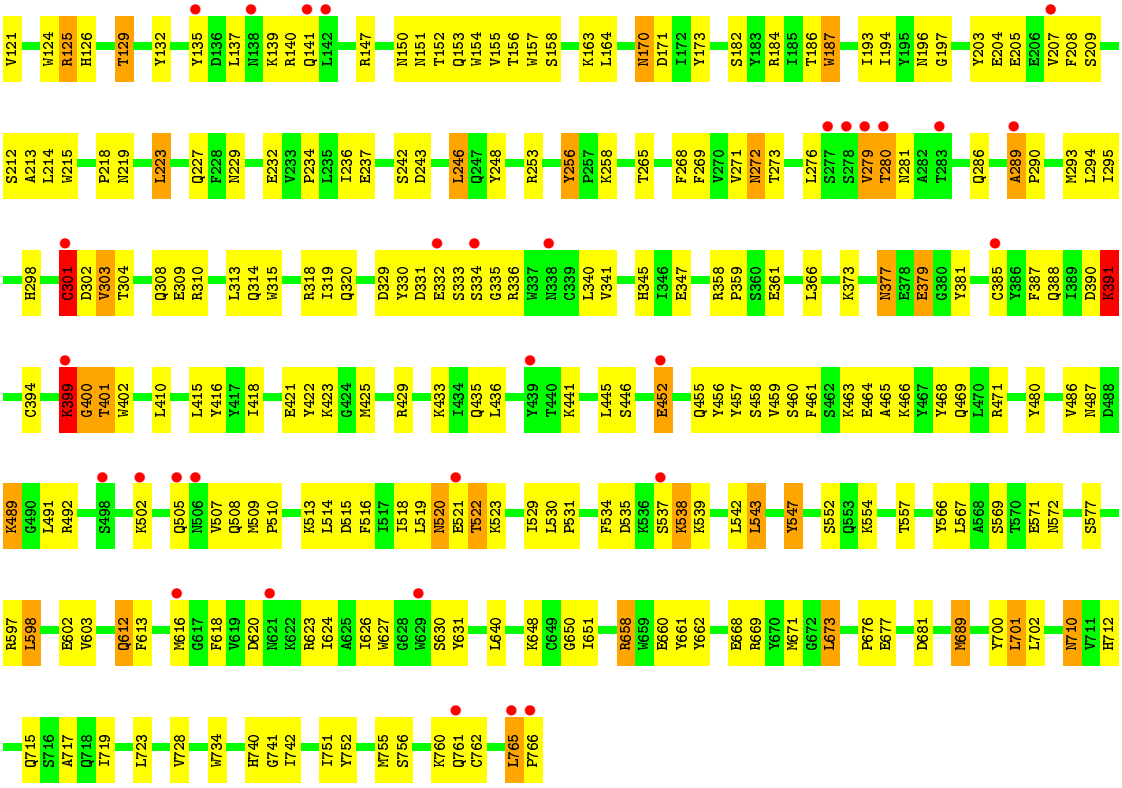
Chain A:



- Molecule 1: Dipeptidyl peptidase

Chain B:




V121 W124 R125 H126 T129 Y132 Y135 D136 L137 N138 K139 R140 Q141 L142 R147 N150 N151 T152 Q153 W154 V155 T156 W157 S158 K163 L164 N170 D171 I172 Y173 S182 Y183 R184 I185 T186 W187 I193 I194 Y195 N196 G197 Y203 E204 E205 E206 V207 F208 S209
S212 A213 L214 W215 P218 N219 L223 Q227 F228 N229 E232 V233 P234 L235 I236 E237 S242 D243 L246 Q247 Y248 R253 Y256 P257 K258 T265 F268 F269 V270 V271 N272 T273 L276 S277 S278 V279 T280 N281 A282 T283 Q286 A289 P290 N293 L294 I295
H298 C301 D302 V303 T304 Q308 E309 R310 L313 Q314 W315 R318 I319 Q320 D329 Y330 D331 E332 S333 S334 G335 R336 W337 N338 C339 L340 V341 H345 I346 E347 R358 P359 S360 E361 L366 K373 N377 E378 E379 G380 Y381 C385 Y386 F387 Q388 I389 D390 K391
C394 R399 G400 T401 W402 L410 L415 Y416 Y417 I418 E421 Y422 K423 G424 M425 R429 K433 I434 Q435 L436 Y439 T440 K441 L445 S446 E452 Q455 Y456 Y457 S458 V459 S460 F461 S462 K463 E464 A465 K466 Y467 Y468 Q469 L470 R471 Y480 V486 N487 D488
K489 G490 L491 R492 S498 K502 Q505 N506 V507 Q508 M509 P510 K513 L514 D515 F516 I517 I518 L519 N520 E521 T522 K523 I529 L530 P531 F534 D535 K536 S537 K538 K539 L542 L543 Y547 S552 Q553 K554 T557 Y566 L567 A568 S569 T570 E571 N572 S577
R597 L598 E602 V603 Q612 F613 M616 G617 F618 V619 D620 N621 K622 R623 I624 A625 I626 W627 G628 W629 S630 Y631 L640 K648 C649 G650 I651 R658 W659 E660 Y661 Y662 E668 R669 Y670 M671 G672 L673 P676 E677 D681 M689 Y700 L701 L702 N710 V711 H712
Q715 S716 A717 Q718 T719 L723 V728 W734 H740 G741 I742 I751 Y752 M755 S756 K760 Q761 C762 L765 P766

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.53 (at 2.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.268 0.229 , 0.265	Depositor DCC
R_{free} test set	4231 reflections (5.34%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 83448 reflections (0.002%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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:218:PRO:HG2	1:B:308:GLN:OE1	1.84	0.78
1:B:184:ARG:HD3	1:B:186:THR:O	1.81	0.78
1:A:630:SER:HG	1:A:740:HIS:HE2	1.31	0.78
1:A:139:LYS:HG3	1:A:141:GLN:HB2	1.66	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:B:207:VAL:HG23	1:B:208:PHE:N	2.08	0.68
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.28	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:B:280:THR:HG23	1:B:281:ASN:N	2.09	0.67
1:A:207:VAL:HG22	1:A:208:PHE:CD1	2.29	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:415:LEU:HD13	3:A:1002:HOH:O	1.95	0.67
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.60	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:HD22	1:B:377:ASN:C	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:B:280:THR:HG23	1:B:281:ASN:H	1.63	0.64
1:A:544:LEU:HD21	1:A:606:GLN:HG3	1.79	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:B:51:ASN:HD21	1:B:54:ARG:CD	2.12	0.63
1:A:522:THR:HG21	1:A:590:ILE:HD11	1.81	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:B:620:ASP:OD2	1:B:623:ARG:HD3	2.00	0.62
1:B:58:TYR:HD1	1:B:60:LEU:HD11	1.65	0.62
1:A:528:MET:HE2	1:A:574:ILE:HG21	1.82	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:177:GLU:CB	1:A:180:LEU:HD13	2.28	0.61
1:A:152:THR:HG21	1:A:155:VAL:CG2	2.29	0.61
1:B:126:HIS:HD2	3:B:905:HOH:O	1.83	0.61
1:B:400:GLY:HA2	3:B:1040:HOH:O	2.00	0.61
1:B:139:LYS:HG3	1:B:141:GLN:HB2	1.81	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: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:A:55:LEU:CD1	1:A:561:LEU:HD22	2.31	0.60
1:B:723:LEU:HB3	1:B:728:VAL:HG13	1.84	0.60
1:B:415:LEU:HD23	1:B:415:LEU:C	2.22	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:392:LYS:HE3	1:A:393:ASP:OD2	2.03	0.59
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.37	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:658:ARG:HG2	1:A:661:TYR:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:HD11	1:A:317:ARG:HH21	1.68	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:89:PHE:CD1	1:A:90:LEU:HD12	2.33	0.57
1:A:306:ALA:HB3	1:A:310:ARG:HB3	1.86	0.57
1:B:69:LEU:CD1	1:B:76:ILE:HD11	2.25	0.57
1:B:445:LEU:HD22	1:B:445:LEU:N	2.19	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:B:293:MET:HE3	1:B:315:TRP:O	2.03	0.57
1:A:603:VAL:HG23	1:A:639:VAL:HG22	1.85	0.57
1:A:581:ARG:HG2	1:A:593:ALA:CB	2.35	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:150:ASN:HA	3:B:937:HOH:O	2.04	0.56
1:B:147:ARG:HB3	1:B:147:ARG:NH1	2.19	0.56
1:A:76:ILE:HB	1:A:90:LEU:HD11	1.87	0.56
1:B:60:LEU:HD13	1:B:469:GLN:CD	2.26	0.56
1:A:205:GLU:OE2	2:A:767:U1N:H111	2.05	0.56
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.35	0.56
1:A:143:ILE:HD12	1:A:143:ILE:H	1.71	0.56
1:A:116:LEU:O	1:A:132:TYR:HA	2.05	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: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:B:765:LEU:CB	1:B:766:PRO:CA	2.84	0.56
1:B:673:LEU:HD22	3:B:1010:HOH:O	2.06	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:40:ARG:CG	1:B:508:GLN:HG3	2.37	0.54
1:B:358:ARG:NH1	1:B:358:ARG:HG2	2.21	0.54
1:A:39:SER:O	1:A:40:ARG:HB2	2.08	0.54
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.43	0.54
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.43	0.54
1:B:78:VAL:HG13	1:B:78:VAL:O	2.07	0.54
1:A:100:HIS:CD2	3:A:917:HOH:O	2.60	0.54
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.43	0.54
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.89	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:B:630:SER:OG	1:B:740:HIS:NE2	2.27	0.53
1:A:581:ARG:HG2	1:A:593:ALA:HB1	1.91	0.53
1:A:658:ARG:HD3	1:A:660:GLU:HB2	1.91	0.53
1:A:40:ARG:HB3	1:A:506:ASN:O	2.07	0.53
1:B:459:VAL:HG22	1:B:460:SER:N	2.23	0.53
1:A:528:MET:CE	1:A:574:ILE:HG21	2.37	0.53
1:A:317:ARG:HG2	3:A:954:HOH:O	2.09	0.53
1:A:269:PHE:CE2	1:A:286:GLN:HB2	2.44	0.53
1:A:603:VAL:HG23	1:A:639:VAL:CG2	2.39	0.53
1:A:143:ILE:HG23	1:A:145:GLU:OE2	2.09	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:286:GLN:HG2	1:A:288:THR:HG22	1.91	0.52
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.10	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:76:ILE:CG2	1:B:90:LEU:HB2	2.39	0.52
1:B:630:SER:HG	1:B:740:HIS:CE1	2.27	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:B:651:ILE:CG2	1:B:755:MET:HE3	2.25	0.51
1:B:147:ARG:HH11	1:B:147:ARG:HB3	1.75	0.51
1:A:96:ASP:C	1:A:98:PHE:H	2.14	0.51
1:A:377:ASN:HB2	1:A:381:TYR:O	2.10	0.51
1:B:391:LYS:HD3	3:B:889:HOH:O	2.11	0.51
1:B:390:ASP:O	1:B:390:ASP:CG	2.48	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: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:65:ASP:OD2	1:A:466:LYS:HB2	2.10	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:765:LEU:HB3	1:B:766:PRO:C	2.31	0.50
1:B:487:ASN:OD1	1:B:489:LYS:HB3	2.11	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:77:LEU:HD22	1:B:88:VAL:HA	1.93	0.50
1:B:289:ALA:HB3	3:B:964:HOH:O	2.11	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:B:157:TRP:CZ3	1:B:164:LEU:HG	2.47	0.50
1:A:741:GLY:O	1:A:742:ILE:C	2.48	0.50
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.94	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:392:LYS:CD	1:A:393:ASP:N	2.60	0.50
1:A:114:ILE:HD12	1:A:137:LEU:HD21	1.92	0.50
1:B:377:ASN:ND2	1:B:381:TYR:H	2.09	0.50
1:A:143:ILE:HD12	1:A:143:ILE:N	2.27	0.50
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.46	0.50
1:B:39:SER:O	1:B:40:ARG:HB3	2.12	0.50
1:B:51:ASN:ND2	1:B:54:ARG:HD3	2.25	0.50
1:B:518:ILE:CD1	1:B:523:LYS:HB3	2.41	0.50
1:A:546:VAL:CG2	1:A:547:TYR:N	2.74	0.50
1:B:455:GLN:HG2	3:B:935:HOH:O	2.12	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:69:LEU:HB3	1:B:76:ILE:HD11	1.94	0.49
1:B:129:THR:OG1	1:B:151:ASN:HA	2.12	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:B:243:ASP:HB3	3:B:849:HOH:O	2.12	0.49
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.76	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:58:TYR:HD1	1:B:60:LEU:CD1	2.25	0.49
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.94	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: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:A:502:LYS:O	1:A:505:GLN:HG2	2.13	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:B:173:TYR:CE2	1:B:184:ARG:HG3	2.49	0.48
1:B:154:TRP:NE1	1:B:156:THR:HG23	2.29	0.48
1:A:458:SER:HB2	1:A:471:ARG:HH21	1.79	0.48
1:B:399:LYS:HD2	1:B:421:GLU:OE2	2.13	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:A:154:TRP:CD1	1:A:214:LEU:HD11	2.48	0.48
1:B:334:SER:OG	1:B:336:ARG:HG2	2.14	0.48
1:A:259:ALA:HB3	1:A:660:GLU:HA	1.95	0.48
1:A:136:ASP:O	1:A:140:ARG:HA	2.14	0.48
1:B:197:GLY:C	1:B:213:ALA:HB3	2.35	0.48
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:681:ASP:HB2	3:A:1031:HOH:O	2.13	0.47
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.95	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:648:LYS:HE2	1:B:762:CYS:O	2.14	0.47
1:B:124:TRP:HB2	1:B:204:GLU:OE2	2.14	0.47
1:B:74:ASN:HB3	1:B:92:ASN:OD1	2.15	0.47
1:B:760:LYS:HB2	1:B:765:LEU:HB2	1.96	0.47
1:B:280:THR:CG2	1:B:281:ASN:N	2.76	0.47
1:A:492:ARG:HG2	1:A:492:ARG:NH1	2.30	0.47
1:B:318:ARG:HG2	3:B:807:HOH:O	2.14	0.47
1:A:739:ASP:HB2	3:A:774:HOH:O	2.13	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:B:538:LYS:HE3	1:B:538:LYS:HA	1.95	0.47
1:A:543:LEU:HD12	1:A:567:LEU:HD13	1.96	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: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:272:ASN:C	1:A:272:ASN:HD22	2.19	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:127:SER:O	1:A:128:TYR:HB3	2.16	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:40:ARG:HH11	1:B:40:ARG:HG2	1.81	0.46
1:B:377:ASN:HD21	1:B:381:TYR:H	1.64	0.46
1:B:293:MET:HG3	1:B:298:HIS:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:TYR:CD1	1:B:60:LEU:HD11	2.46	0.46
1:A:93:SER:HA	1:A:96:ASP:OD1	2.16	0.46
1:A:390:ASP:OD1	1:A:391:LYS:HD3	2.16	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:571:GLU:HB3	1:B:765:LEU:HD21	1.98	0.45
1:B:543:LEU:HD12	1:B:567:LEU:HD13	1.99	0.45
1:B:223:LEU:HB3	1:B:271:VAL:HG12	1.99	0.45
1:B:280:THR:CG2	1:B:281:ASN:H	2.26	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: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: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:142:LEU:O	1:A:144:THR:HG23	2.16	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:B:751:ILE:O	1:B:755:MET:HG3	2.16	0.45
1:A:76:ILE:HB	1:A:90:LEU:HD13	1.98	0.45
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.99	0.45
1:A:217:SER:HB3	1:A:222:PHE:HB2	1.99	0.45
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.52	0.45
1:B:268:PHE:CD2	1:B:313:LEU:HD21	2.52	0.45
1:B:258:LYS:NZ	1:B:712:HIS:CD2	2.78	0.45
1:A:242:SER:OG	1:A:243:ASP:N	2.48	0.45
1:A:77:LEU:CD2	1:A:88:VAL:HG22	2.47	0.44
1:B:289:ALA:HB1	1:B:290:PRO:C	2.38	0.44
1:A:105:TYR:CD1	1:A:105:TYR:N	2.85	0.44
1:A:154:TRP:HE1	1:A:214:LEU:HD11	1.82	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:B:538:LYS:HD3	1:B:539:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD12	1:A:343:ARG:HD2	1.99	0.44
1:A:492:ARG:HH11	1:A:492:ARG:HG2	1.82	0.44
1:B:289:ALA:CA	1:B:294:LEU:HD11	2.47	0.44
1:B:281:ASN:ND2	3:B:792:HOH:O	2.50	0.44
1:B:214:LEU:HD12	1:B:214:LEU:O	2.17	0.44
1:B:60:LEU:HD11	1:B:469:GLN:NE2	2.32	0.44
1:A:145:GLU:CG	1:A:179:ASN:HB2	2.48	0.44
1:B:273:THR:HA	1:B:276:LEU:HG	2.00	0.44
1:A:60:LEU:HD12	1:A:60:LEU:O	2.17	0.44
1:B:658:ARG:O	1:B:658:ARG:HG3	2.17	0.43
1:B:547:TYR:CD1	1:B:552:SER:HB2	2.53	0.43
1:B:418:ILE:CG2	1:B:429:ARG:HG3	2.48	0.43
1:A:542:LEU:HD23	1:A:542:LEU:C	2.39	0.43
1:B:662:TYR:OH	1:B:710:ASN:ND2	2.47	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: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:140:ARG:HG2	1:A:140:ARG:NH1	2.29	0.43
1:B:489:LYS:HG3	1:B:489:LYS:O	2.17	0.43
1:A:280:THR:HG22	1:A:281:ASN:N	2.34	0.43
1:A:63:ILE:CG2	1:A:69:LEU:HG	2.49	0.43
1:A:295:ILE:CD1	1:A:317:ARG:HH21	2.31	0.43
1:B:385:CYS:SG	1:B:387:PHE:CE2	3.11	0.43
1:A:612:GLN:HB3	1:A:612:GLN:HE21	1.53	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:B:237:GLU:HG2	1:B:253:ARG:HG2	2.00	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:446:SER:HB2	1:B:457:TYR:CE2	2.54	0.43
1:B:51:ASN:HD21	1:B:54:ARG:HG3	1.83	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:A:489:LYS:NZ	3:A:1013:HOH:O	2.50	0.43
1:B:74:ASN:O	1:B:92:ASN:HA	2.18	0.43
1:A:41:LYS:O	1:A:508:GLN:N	2.44	0.43
1:A:273:THR:HA	1:A:276:LEU:HD22	2.01	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:A:458:SER:OG	1:A:471:ARG:HB2	2.19	0.43
1:B:515:ASP:CG	1:B:516:PHE:H	2.22	0.43
1:B:51:ASN:HD21	1:B:54:ARG:CG	2.32	0.43
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.94	0.43
1:A:325:MET:CE	1:A:327:ILE:HD11	2.49	0.42
1:B:723:LEU:CD2	1:B:728:VAL:HG11	2.48	0.42
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.39	0.42
1:A:626:ILE:O	1:A:650:GLY:HA2	2.18	0.42
1:A:171:ASP:OD1	1:A:186:THR:HG23	2.19	0.42
1:B:723:LEU:O	1:B:728:VAL:HG12	2.19	0.42
1:A:568:ALA:HA	1:A:573:ILE:O	2.19	0.42
1:B:571:GLU:OE1	1:B:765:LEU:HD23	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:648:LYS:HD3	1:B:762:CYS:SG	2.59	0.42
1:B:347:GLU:OE1	1:B:373:LYS:NZ	2.48	0.42
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.02	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:A:172:ILE:N	1:A:186:THR:HG22	2.19	0.42
1:A:415:LEU:C	1:A:415:LEU:CD1	2.87	0.42
1:B:518:ILE:HD11	1:B:523:LYS:HB3	2.01	0.42
1:B:491:LEU:O	1:B:492:ARG:HB3	2.19	0.42
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.55	0.42
1:B:734:TRP:CD1	1:B:734:TRP:C	2.93	0.42
1:A:319:ILE:C	1:A:321:ASN:H	2.22	0.42
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.55	0.42
1:A:62:TRP:HB3	3:A:901:HOH:O	2.18	0.42
1:A:607:ILE:HG22	1:A:611:ARG:NH1	2.34	0.42
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.19	0.42
1:B:518:ILE:HD13	1:B:523:LYS:HA	2.02	0.42
1:B:651:ILE:HG23	1:B:701:LEU:HB3	2.02	0.42
1:A:134:ILE:O	1:A:143:ILE:HD13	2.19	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:A:344:GLN:HE21	1:A:346:ILE:HD11	1.85	0.42
1:A:691:ARG:HG3	1:A:691:ARG:HH11	1.85	0.42
1:B:612:GLN:HE21	1:B:612:GLN:HB3	1.59	0.42
1:B:116:LEU:O	1:B:132:TYR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:SER:HB3	1:A:163:LYS:HB2	2.02	0.42
1:A:518:ILE:C	3:A:1001:HOH:O	2.58	0.41
1:B:86:SER:O	1:B:87:SER:HB3	2.20	0.41
1:A:96:ASP:O	1:A:98:PHE:N	2.53	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:529:ILE:HD11	3:B:848:HOH:O	2.20	0.41
1:B:215:TRP:CE2	1:B:303:VAL:CG1	3.03	0.41
1:A:177:GLU:HB2	1:A:180:LEU:CD1	2.39	0.41
1:A:736:THR:HG23	3:B:793:HOH:O	2.19	0.41
1:A:463:LYS:NZ	3:A:901:HOH:O	2.54	0.41
1:B:75:ASN:HD22	1:B:92:ASN:HB2	1.85	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:B:658:ARG:HD3	1:B:660:GLU:HB2	2.01	0.41
1:A:531:PRO:HA	1:A:532:PRO:HD3	1.90	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:B:69:LEU:HA	1:B:77:LEU:O	2.21	0.41
1:B:571:GLU:HB3	1:B:765:LEU:CD2	2.51	0.41
1:B:538:LYS:HE3	1:B:539:LYS:N	2.32	0.41
1:A:543:LEU:HD23	1:A:544:LEU:N	2.36	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.41
1:B:433:LYS:HB3	1:B:445:LEU:HD21	2.02	0.41
1:B:518:ILE:HD13	1:B:523:LYS:HB3	2.02	0.41
1:B:154:TRP:CE2	1:B:156:THR:HG23	2.56	0.41
1:A:513:LYS:HE3	1:A:530:LEU:HD11	2.03	0.41
1:A:726:VAL:O	1:A:726:VAL:HG13	2.21	0.41
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.56	0.41
1:B:256:TYR:CD1	1:B:256:TYR:C	2.94	0.41
1:B:751:ILE:HG23	1:B:752:TYR:N	2.35	0.41
1:B:60:LEU:HD12	1:B:60:LEU:N	2.36	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:193:ILE:HG22	1:B:194:ILE:HG12	2.02	0.40
1:A:139:LYS:CD	1:A:141:GLN:HB2	2.52	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:236:ILE:HG22	1:A:254:VAL:O	2.22	0.40
1:B:207:VAL:CG2	1:B:208:PHE:H	2.33	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:B:542:LEU:O	1:B:624:ILE:HA	2.21	0.40
1:A:507:VAL:CG2	1:A:509:MET:HG2	2.52	0.40
1:B:681:ASP:HB2	3:B:1032:HOH:O	2.22	0.40
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.56	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: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:392:LYS:HD2	1:A:393:ASP:CA	2.48	0.40
1:A:139:LYS:HG3	1:A:141:GLN:H	1.86	0.40
1:B:39:SER:O	1:B:40:ARG:CB	2.70	0.40
1:A:720:SER:O	1:A:724:VAL:HG23	2.21	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%)	17	11
1	B	726/728 (100%)	662 (91%)	56 (8%)	8 (1%)	17	11
All	All	1450/1456 (100%)	1323 (91%)	111 (8%)	16 (1%)	17	11

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 (i)

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%)	16	11
1	B	653/653 (100%)	605 (93%)	48 (7%)	17	13
All	All	1304/1306 (100%)	1205 (92%)	99 (8%)	16	12

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	-	25,25,25	1.98	10 (40%)	32,33,33	1.62	7 (21%)
2	U1N	B	767	-	25,25,25	2.04	11 (44%)	32,33,33	1.59	6 (18%)

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	-	-	0/18/18/18	0/2/2/2
2	U1N	B	767	-	-	1/18/18/18	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	767	U1N	C1-C23	-2.20	1.47	1.50
2	B	767	U1N	C3-C2	2.01	1.42	1.38
2	B	767	U1N	C6-C5	2.02	1.42	1.38
2	A	767	U1N	C3-C4	2.15	1.43	1.38
2	A	767	U1N	C3-C2	2.23	1.42	1.38
2	B	767	U1N	C2-C1	2.25	1.43	1.39
2	B	767	U1N	C18-C19	2.29	1.41	1.37
2	A	767	U1N	C16-C14	2.31	1.53	1.49
2	A	767	U1N	C18-C19	2.34	1.41	1.37
2	A	767	U1N	C21-C19	2.39	1.41	1.37
2	A	767	U1N	C6-C1	2.42	1.43	1.39
2	B	767	U1N	C21-C19	2.48	1.42	1.37
2	B	767	U1N	C18-C17	2.56	1.43	1.38
2	A	767	U1N	C22-C16	2.64	1.43	1.39
2	A	767	U1N	C2-C1	2.69	1.43	1.39
2	B	767	U1N	C6-C1	2.75	1.44	1.39
2	A	767	U1N	C17-C16	2.78	1.44	1.39
2	B	767	U1N	C17-C16	2.83	1.44	1.39
2	B	767	U1N	C22-C16	3.03	1.44	1.39
2	A	767	U1N	C23-N24	4.68	1.42	1.33
2	B	767	U1N	C23-N24	4.98	1.43	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	767	U1N	O25-C23-N24	-4.94	115.65	122.59
2	B	767	U1N	O25-C23-N24	-4.77	115.88	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	767	U1N	C11-C9-C8	-2.84	106.64	111.24
2	A	767	U1N	C11-C9-C8	-2.68	106.91	111.24
2	A	767	U1N	O15-C14-C16	-2.53	116.61	120.71
2	B	767	U1N	O15-C14-C16	-2.38	116.86	120.71
2	A	767	U1N	C13-C14-C16	2.11	120.24	117.85
2	A	767	U1N	O15-C14-C13	2.25	123.14	120.10
2	B	767	U1N	C13-C14-C16	2.30	120.45	117.85
2	B	767	U1N	C1-C23-N24	2.74	120.81	117.82
2	A	767	U1N	C1-C23-N24	3.01	121.11	117.82
2	A	767	U1N	O25-C23-C1	3.35	123.24	119.59
2	B	767	U1N	O25-C23-C1	3.40	123.30	119.59

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	767	U1N	C16-C14-C13-N12

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

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, 95^{th} 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%)	0.53	69 (9%)	10	14	17, 31, 70, 93	0
1	B	728/728 (100%)	0.56	60 (8%)	14	20	18, 31, 62, 87	0
All	All	1454/1456 (99%)	0.55	129 (8%)	12	16	17, 31, 66, 93	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	19.9
1	A	39	SER	11.5
1	B	73	GLU	10.3
1	B	278	SER	9.4
1	B	40	ARG	8.9
1	A	73	GLU	8.3
1	B	97	GLU	8.2
1	B	74	ASN	7.1
1	B	39	SER	7.0
1	A	83	TYR	6.9
1	A	98	PHE	6.4
1	B	277	SER	6.2
1	A	102	ILE	6.1
1	A	90	LEU	6.1
1	A	74	ASN	6.0
1	A	84	GLY	5.9
1	A	71	LYS	5.8
1	A	99	GLY	5.8
1	B	83	TYR	5.7
1	A	76	ILE	5.6
1	A	95	PHE	5.6
1	A	105	TYR	5.5
1	B	766	PRO	5.4
1	A	94	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	139	LYS	5.1
1	A	100	HIS	5.0
1	A	96	ASP	4.8
1	A	101	SER	4.7
1	B	72	GLN	4.6
1	B	91	GLU	4.6
1	B	96	ASP	4.5
1	A	93	SER	4.4
1	B	82	GLU	4.4
1	A	135	TYR	4.3
1	A	138	ASN	4.3
1	A	88	VAL	4.3
1	B	138	ASN	4.2
1	B	765	LEU	4.2
1	A	141	GLN	4.2
1	B	92	ASN	4.2
1	B	99	GLY	4.1
1	B	280	THR	4.0
1	A	103	ASN	3.9
1	B	81	ALA	3.9
1	A	134	ILE	3.9
1	A	87	SER	3.9
1	A	333	SER	3.8
1	B	521	GLU	3.8
1	B	86	SER	3.8
1	A	160	VAL	3.7
1	A	137	LEU	3.7
1	A	92	ASN	3.7
1	A	89	PHE	3.6
1	A	77	LEU	3.6
1	A	91	GLU	3.5
1	B	71	LYS	3.5
1	B	537	SER	3.4
1	B	87	SER	3.3
1	B	616	MET	3.3
1	B	93	SER	3.2
1	A	148	ILE	3.1
1	B	78	VAL	3.1
1	A	70	TYR	3.1
1	A	81	ALA	3.0
1	A	82	GLU	3.0
1	A	279	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	385	CYS	3.0
1	B	334	SER	2.9
1	A	40	ARG	2.9
1	B	289	ALA	2.9
1	A	97	GLU	2.9
1	B	70	TYR	2.9
1	B	505	GLN	2.9
1	B	338	ASN	2.9
1	B	283	THR	2.9
1	A	78	VAL	2.8
1	B	301	CYS	2.8
1	A	332	GLU	2.8
1	A	336	ARG	2.8
1	A	75	ASN	2.7
1	B	141	GLN	2.7
1	A	142	LEU	2.7
1	B	399	LYS	2.7
1	A	114	ILE	2.7
1	A	86	SER	2.7
1	A	289	ALA	2.6
1	B	101	SER	2.6
1	B	88	VAL	2.6
1	A	85	ASN	2.5
1	A	107	ILE	2.5
1	A	342	ALA	2.5
1	B	98	PHE	2.5
1	A	61	ARG	2.5
1	B	76	ILE	2.5
1	B	84	GLY	2.5
1	B	207	VAL	2.5
1	B	621	ASN	2.4
1	A	110	ASP	2.4
1	A	392	LYS	2.4
1	A	69	LEU	2.4
1	A	179	ASN	2.4
1	A	492	ARG	2.4
1	B	506	ASN	2.4
1	A	145	GLU	2.3
1	A	136	ASP	2.3
1	B	89	PHE	2.3
1	A	505	GLN	2.3
1	B	761	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	PHE	2.2
1	A	330	TYR	2.2
1	B	142	LEU	2.2
1	B	135	TYR	2.2
1	A	278	SER	2.2
1	A	140	ARG	2.2
1	A	335	GLY	2.2
1	B	75	ASN	2.2
1	B	94	THR	2.2
1	B	498	SER	2.1
1	A	536	LYS	2.1
1	B	629	TRP	2.1
1	B	332	GLU	2.0
1	B	100	HIS	2.0
1	A	498	SER	2.0
1	A	72	GLN	2.0
1	A	697	GLN	2.0
1	B	90	LEU	2.0
1	B	502	LYS	2.0
1	B	439	TYR	2.0
1	B	452	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	U1N	B	767	24/24	0.89	0.29	5.98	32,48,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	U1N	A	767	24/24	0.87	0.22	4.52	36,46,50,53	0

6.5 Other polymers (i)

There are no such residues in this entry.