



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:57 PM 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 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/ValidationPDFNotes.html>

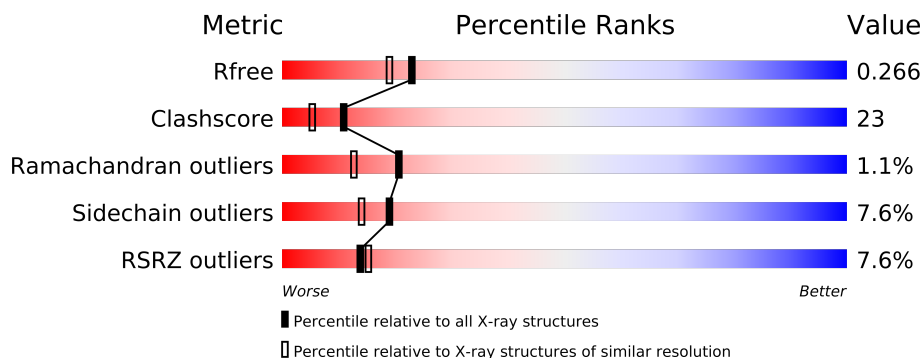
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	728	
1	B	728	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	UIN	A	767	-	X
2	UIN	B	767	-	X

2 Entry composition i

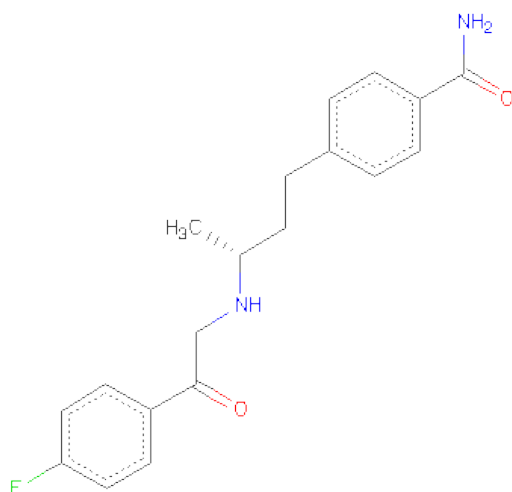
There are 3 unique types of molecules in this entry. The entry contains 12514 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called 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		

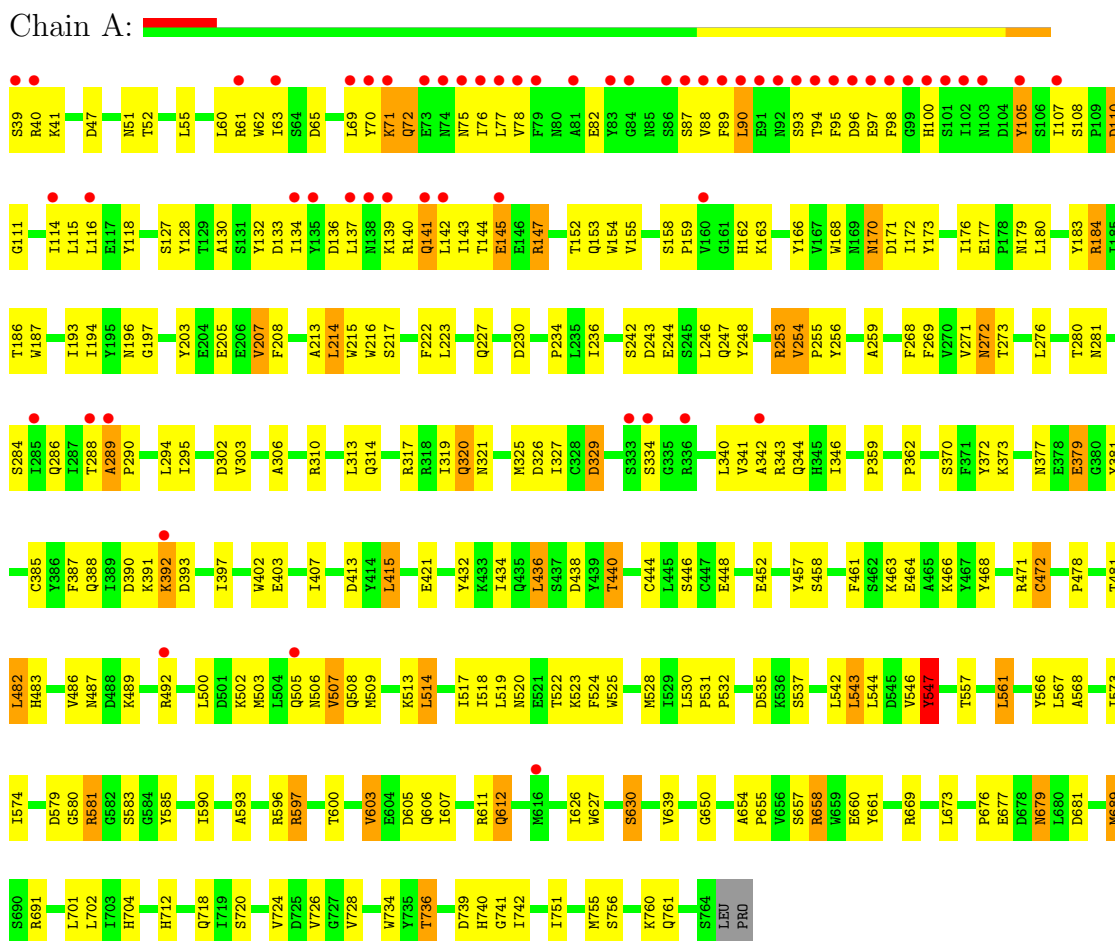
- Molecule 3 is water.

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

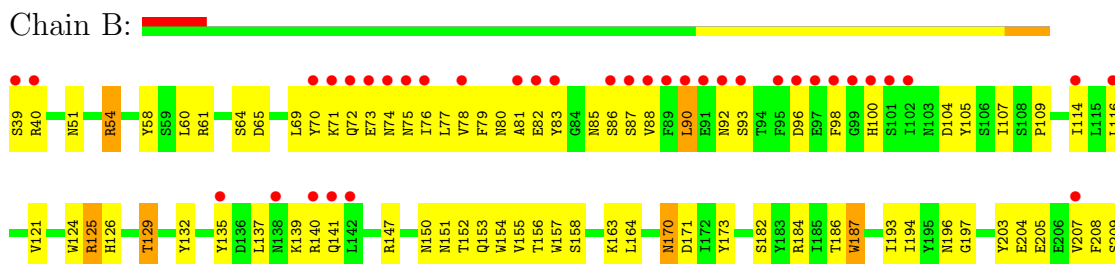
3 Residue-property plots

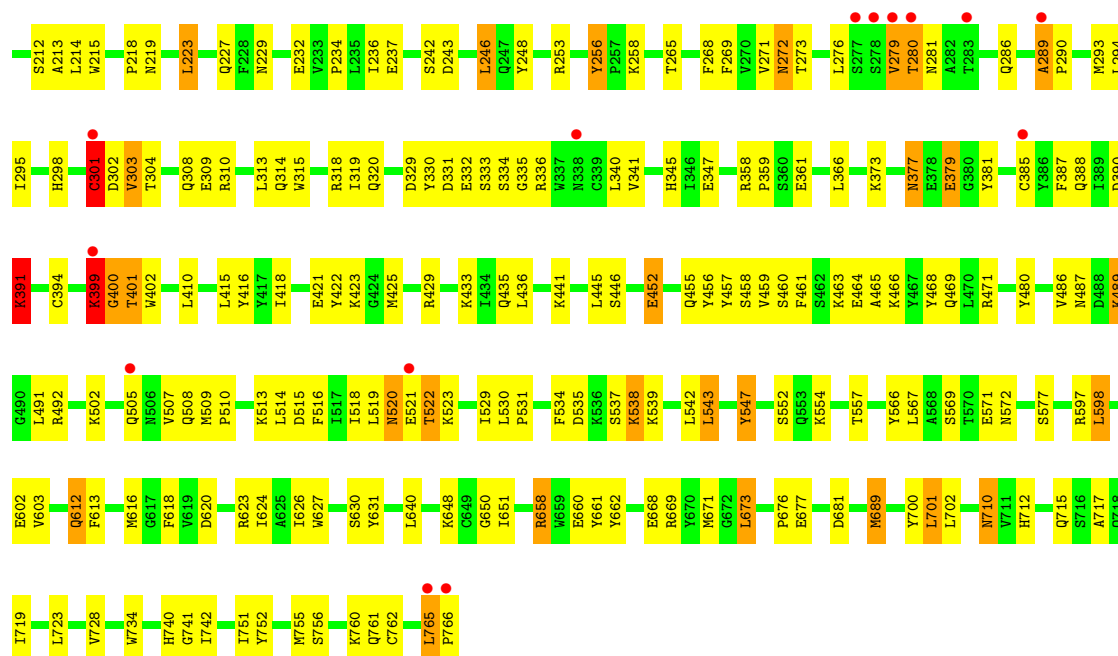
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Dipeptidyl peptidase



• Molecule 1: Dipeptidyl peptidase





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) 86.1 (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 0.230 , 0.266	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)	0.38 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (529) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:B:765:LEU:HB3	1:B:766:PRO:OXT	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	724/728 (100%)	661 (91%)	55 (8%)	8 (1%)	21	13
1	B	726/728 (100%)	662 (91%)	56 (8%)	8 (1%)	21	13
All	All	1450/1456 (100%)	1323 (91%)	111 (8%)	16 (1%)	21	13

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

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Mol	Chain	Res	Type
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%)	18	13
1	B	653/653 (100%)	605 (93%)	48 (7%)	20	15
All	All	1304/1306 (100%)	1205 (92%)	99 (8%)	19	14

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	718	GLN
1	B	731	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	U1N	A	767	-	25,25,25	1.95	10 (40%)	33,33,33	1.61	6 (18%)
2	U1N	B	767	-	25,25,25	1.97	9 (36%)	33,33,33	1.58	7 (21%)

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	-	-	2/18/18/18	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	767	U1N	C23-N24	4.48	1.43	1.33
2	A	767	U1N	C23-N24	4.21	1.42	1.33
2	B	767	U1N	C22-C16	3.00	1.44	1.39
2	B	767	U1N	C17-C16	2.80	1.44	1.39
2	A	767	U1N	C17-C16	2.75	1.44	1.39
2	B	767	U1N	C6-C1	2.72	1.44	1.39
2	A	767	U1N	C2-C1	2.66	1.43	1.39
2	A	767	U1N	C22-C16	2.61	1.43	1.39
2	B	767	U1N	C21-C19	2.60	1.42	1.36
2	A	767	U1N	C13-C14	2.55	1.55	1.51
2	A	767	U1N	C21-C19	2.50	1.41	1.36
2	A	767	U1N	C18-C19	2.45	1.41	1.36
2	A	767	U1N	C6-C1	2.40	1.43	1.39
2	B	767	U1N	C18-C17	2.40	1.43	1.38
2	B	767	U1N	C18-C19	2.39	1.41	1.36
2	A	767	U1N	C16-C14	2.24	1.53	1.49
2	B	767	U1N	C2-C1	2.23	1.43	1.39
2	A	767	U1N	C3-C2	2.09	1.42	1.38
2	B	767	U1N	C1-C23	-2.04	1.47	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	767	U1N	O25-C23-N24	-4.81	115.65	122.59
2	B	767	U1N	O25-C23-N24	-4.64	115.88	122.59
2	B	767	U1N	O25-C23-C1	3.30	123.30	119.58
2	A	767	U1N	O25-C23-C1	3.25	123.24	119.58
2	A	767	U1N	C1-C23-N24	2.94	121.11	117.77
2	B	767	U1N	C11-C9-C8	-2.91	106.64	111.31
2	A	767	U1N	C11-C9-C8	-2.75	106.91	111.31
2	B	767	U1N	C1-C23-N24	2.67	120.81	117.77
2	A	767	U1N	O15-C14-C16	-2.50	116.61	120.68
2	B	767	U1N	O15-C14-C16	-2.34	116.86	120.68
2	A	767	U1N	O15-C14-C13	2.24	123.14	120.43
2	B	767	U1N	C13-C14-C16	2.15	120.45	117.95
2	B	767	U1N	C7-C8-C9	2.11	115.75	112.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	767	U1N	O15-C14-C13-N12
2	B	767	U1N	C16-C14-C13-N12

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.38	59 (8%) 12 13	17, 31, 70, 93	0
1	B	728/728 (100%)	0.38	51 (7%) 16 18	18, 31, 62, 87	0
All	All	1454/1456 (99%)	0.38	110 (7%) 14 15	17, 31, 66, 93	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	17.0
1	A	39	SER	9.1
1	B	40	ARG	8.1
1	B	73	GLU	7.5
1	B	278	SER	7.5
1	A	71	LYS	7.5
1	A	76	ILE	7.2
1	A	73	GLU	7.0
1	A	105	TYR	6.9
1	A	102	ILE	6.6
1	B	97	GLU	6.5
1	B	39	SER	6.2
1	A	98	PHE	5.9
1	A	95	PHE	5.8
1	B	74	ASN	5.8
1	A	90	LEU	5.7
1	B	99	GLY	5.5
1	B	71	LYS	5.1
1	A	83	TYR	5.0
1	B	277	SER	4.9
1	A	94	THR	4.9
1	A	139	LYS	4.7
1	B	72	GLN	4.6
1	A	77	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	84	GLY	4.4
1	B	83	TYR	4.2
1	B	98	PHE	4.2
1	A	137	LEU	4.1
1	B	86	SER	4.1
1	A	138	ASN	4.0
1	A	89	PHE	4.0
1	B	765	LEU	4.0
1	A	100	HIS	3.9
1	B	766	PRO	3.8
1	B	89	PHE	3.8
1	A	78	VAL	3.7
1	A	74	ASN	3.7
1	B	521	GLU	3.6
1	B	91	GLU	3.6
1	B	90	LEU	3.5
1	A	99	GLY	3.4
1	A	135	TYR	3.4
1	A	333	SER	3.4
1	B	76	ILE	3.4
1	B	92	ASN	3.3
1	B	95	PHE	3.3
1	A	141	GLN	3.3
1	B	70	TYR	3.3
1	A	96	ASP	3.3
1	B	78	VAL	3.3
1	A	87	SER	3.3
1	A	103	ASN	3.2
1	B	141	GLN	3.2
1	A	70	TYR	3.1
1	A	107	ILE	3.1
1	A	101	SER	3.0
1	B	142	LEU	3.0
1	A	40	ARG	3.0
1	B	138	ASN	3.0
1	B	96	ASP	2.9
1	A	114	ILE	2.9
1	B	88	VAL	2.9
1	A	289	ALA	2.9
1	A	134	ILE	2.9
1	B	87	SER	2.9
1	B	338	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	102	ILE	2.9
1	A	142	LEU	2.9
1	A	336	ARG	2.8
1	B	207	VAL	2.8
1	A	342	ALA	2.8
1	A	93	SER	2.8
1	B	101	SER	2.8
1	B	93	SER	2.8
1	A	97	GLU	2.8
1	B	280	THR	2.7
1	A	145	GLU	2.7
1	B	100	HIS	2.7
1	B	114	ILE	2.6
1	A	392	LYS	2.6
1	A	616	MET	2.5
1	B	82	GLU	2.5
1	B	289	ALA	2.5
1	A	79	PHE	2.5
1	A	160	VAL	2.5
1	B	385	CYS	2.5
1	A	75	ASN	2.4
1	A	69	LEU	2.4
1	A	81	ALA	2.4
1	B	399	LYS	2.3
1	A	88	VAL	2.3
1	B	283	THR	2.3
1	A	63	ILE	2.3
1	A	91	GLU	2.3
1	B	81	ALA	2.3
1	B	505	GLN	2.3
1	A	92	ASN	2.3
1	A	86	SER	2.2
1	B	135	TYR	2.2
1	A	492	ARG	2.2
1	A	61	ARG	2.2
1	A	505	GLN	2.2
1	A	288	THR	2.2
1	B	301	CYS	2.1
1	A	116	LEU	2.1
1	A	285	ILE	2.1
1	B	116	LEU	2.1
1	B	140	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	75	ASN	2.0
1	A	334	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	U1N	B	767	24/24	0.27	5.05	32,48,56,56	0
2	U1N	A	767	24/24	0.21	3.84	36,46,50,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.