



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 2OGZ / pdb_00002ogz
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

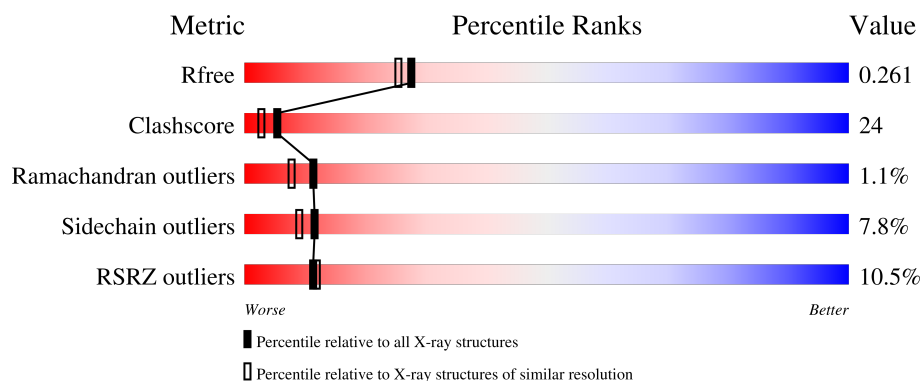
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of 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	11% 58% 35% 6% •
1	B	728	10% 59% 34% 6% •

2 Entry composition [i](#)

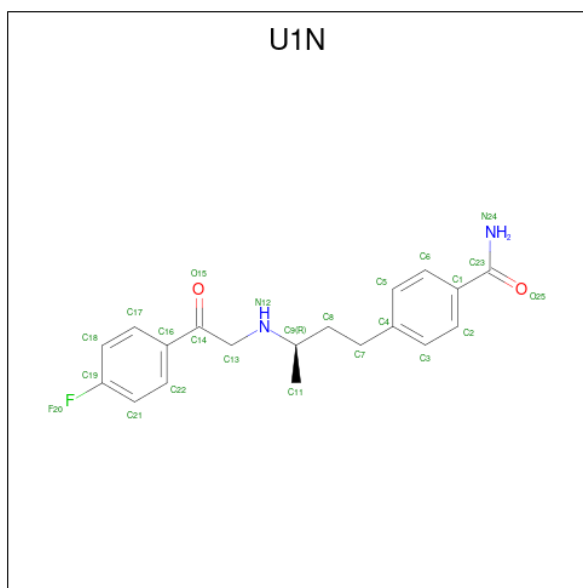
There are 3 unique types of molecules in this entry. The entry contains 12514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

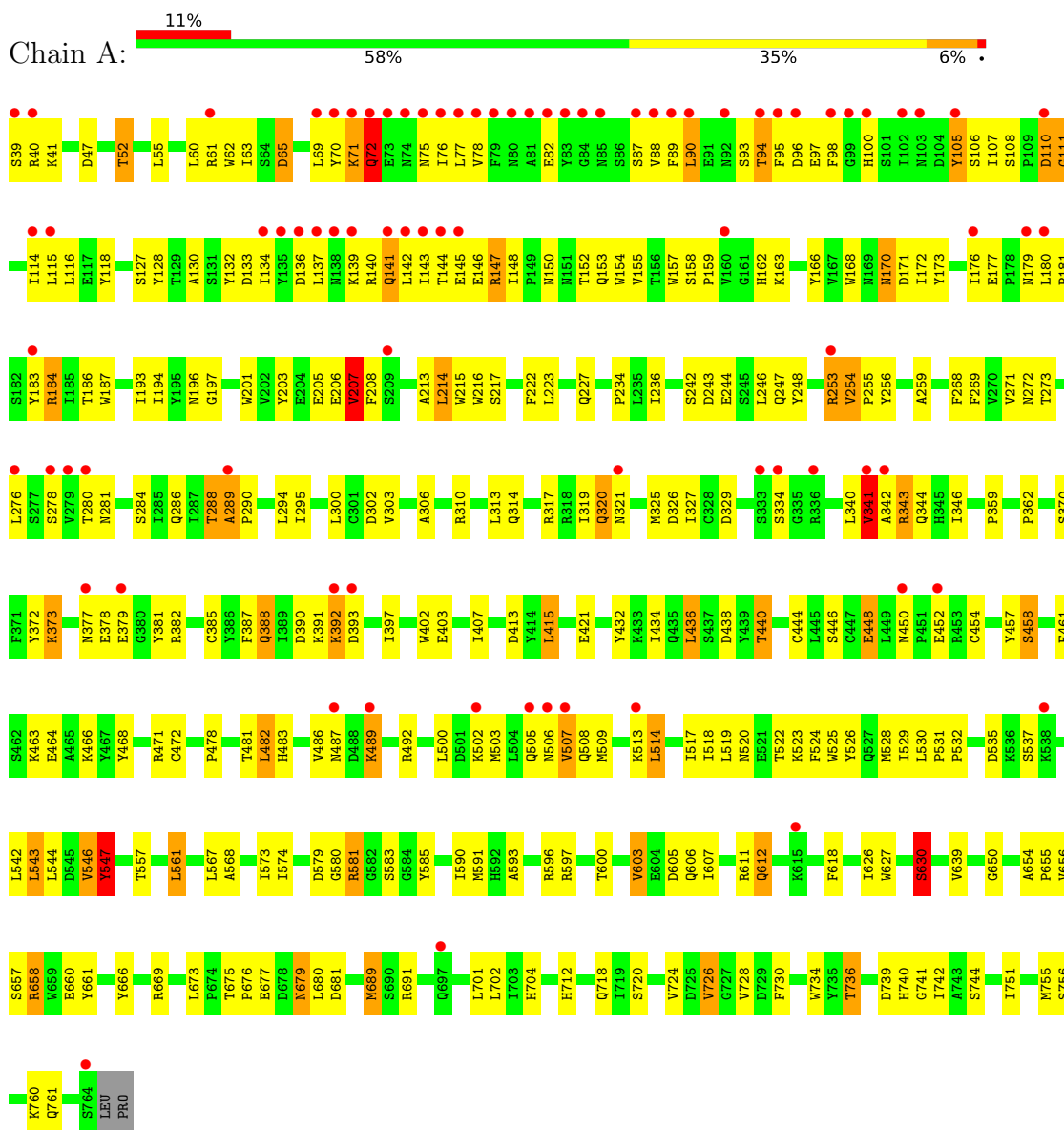
- Molecule 3 is water.

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 [i](#)

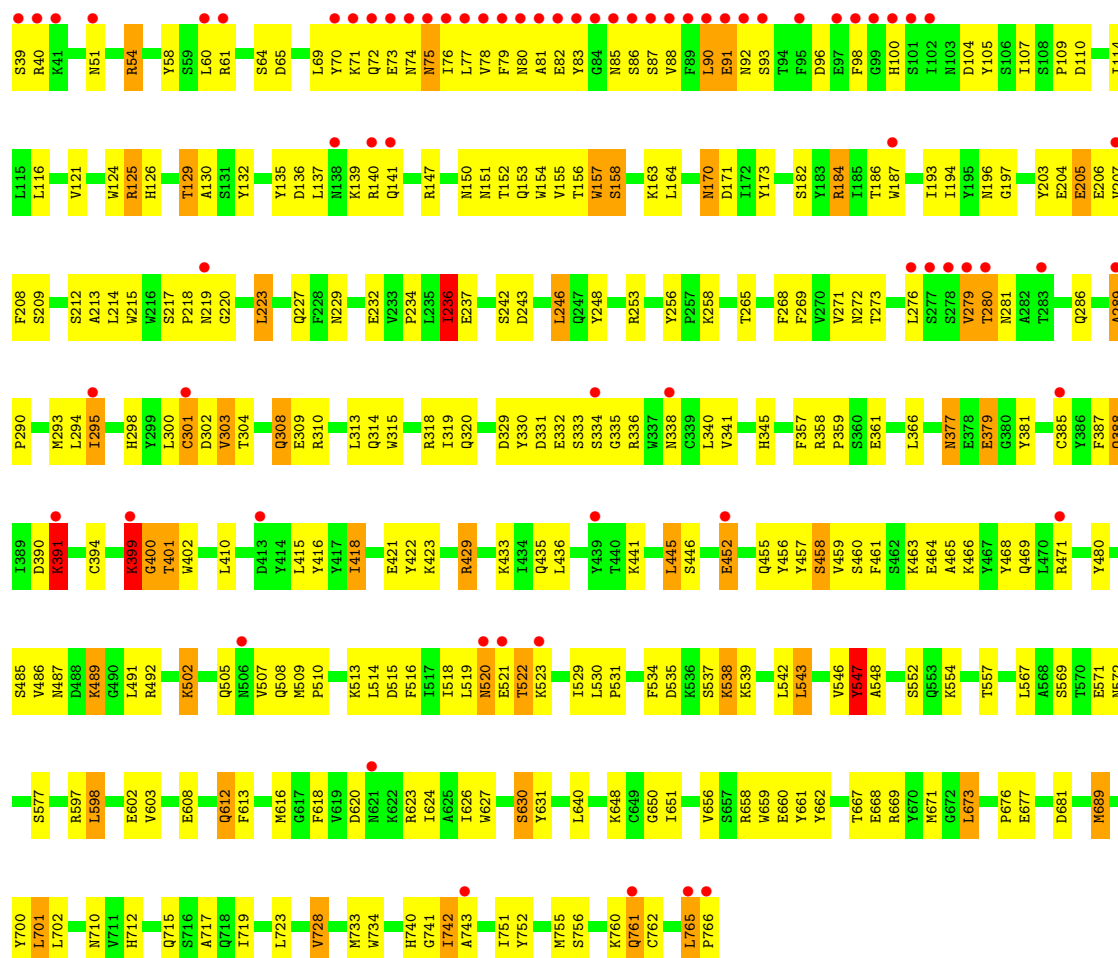
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• 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 50.00 – 2.11	Depositor EDS
% Data completeness (in resolution range)	84.4 (50.00-2.10) 86.1 (50.00-2.11)	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 0.225 , 0.261	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)	0.35 , 38.4	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

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	0.41	0/6119	0.97	27/8321 (0.3%)
1	B	0.42	0/6136	0.95	24/8344 (0.3%)
All	All	0.42	0/12255	0.96	51/16665 (0.3%)

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

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	378	GLU	N-CA-C	-8.73	102.06	112.89
1	A	206	GLU	N-CA-C	8.59	123.88	113.23
1	B	319	ILE	N-CA-C	-7.49	96.73	107.37
1	A	546	VAL	N-CA-C	7.03	119.68	108.85
1	B	399	LYS	N-CA-C	7.01	125.74	110.80
1	B	630	SER	CB-CA-C	-7.01	107.69	117.23
1	A	388	GLN	N-CA-C	-6.98	97.52	108.90
1	B	485	SER	N-CA-C	6.91	120.81	112.38
1	A	630	SER	CB-CA-C	-6.69	108.13	117.23
1	A	207	VAL	N-CA-C	6.67	116.89	111.62
1	B	546	VAL	N-CA-C	6.62	119.05	108.85
1	B	206	GLU	N-CA-C	6.57	122.26	113.72
1	A	454	CYS	N-CA-C	6.50	119.00	108.34
1	A	450	ASN	CA-C-N	6.38	126.87	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ASN	C-N-CA	6.38	126.87	119.47
1	B	220	GLY	N-CA-C	-6.26	106.45	115.27
1	A	547	TYR	N-CA-C	-6.25	97.48	110.80
1	A	744	SER	N-CA-C	-6.18	101.79	110.50
1	B	656	VAL	N-CA-C	-6.17	99.37	109.12
1	B	458	SER	N-CA-C	-6.05	100.10	109.24
1	A	111	GLY	N-CA-C	-6.05	107.05	114.92
1	A	150	ASN	N-CA-C	-6.04	102.98	110.41
1	B	548	ALA	N-CA-C	6.02	119.85	111.90
1	B	236	ILE	N-CA-C	-6.00	99.94	108.58
1	B	300	LEU	N-CA-C	-5.97	99.46	108.96
1	A	278	SER	N-CA-C	-5.96	104.47	113.89
1	B	659	TRP	N-CA-C	5.87	118.45	111.71
1	A	448	GLU	N-CA-C	5.84	120.40	113.16
1	A	458	SER	N-CA-C	-5.74	100.59	109.14
1	B	400	GLY	N-CA-C	5.49	126.19	113.18
1	B	157	TRP	N-CA-C	-5.45	103.33	110.53
1	A	300	LEU	N-CA-C	-5.39	98.44	107.99
1	B	205	GLU	N-CA-C	5.37	116.94	111.14
1	A	343	ARG	N-CA-C	-5.28	106.86	113.72
1	B	667	THR	N-CA-C	5.26	116.70	110.97
1	A	341	VAL	N-CA-C	-5.25	98.42	109.34
1	A	148	ILE	CA-C-N	5.22	125.22	119.90
1	A	148	ILE	C-N-CA	5.22	125.22	119.90
1	A	529	ILE	N-CA-C	-5.19	99.63	107.73
1	B	357	PHE	N-CA-C	-5.19	106.91	114.12
1	A	656	VAL	N-CA-C	-5.18	101.00	108.87
1	B	217	SER	N-CA-C	-5.15	102.98	110.08
1	B	388	GLN	N-CA-C	-5.14	101.31	109.59
1	A	65	ASP	N-CA-C	-5.12	107.08	113.38
1	B	130	ALA	N-CA-C	5.08	116.02	108.60
1	A	201	TRP	N-CA-C	5.07	117.19	111.11
1	B	158	SER	N-CA-C	-5.06	102.80	110.39
1	B	91	GLU	N-CA-C	5.05	116.62	110.41
1	B	547	TYR	N-CA-C	-5.01	100.13	110.80
1	A	206	GLU	CA-C-N	-5.00	117.86	123.16
1	A	206	GLU	C-N-CA	-5.00	117.86	123.16

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	283	0
1	B	5964	0	5685	286	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	557	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 24.

All (557) 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: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:500:LEU:HA	1:A:503:MET:HE3	1.46	0.96
1:B:651:ILE:HG21	1:B:755:MET:HE3	1.50	0.94
1:B:219:ASN:HB2	1:B:308:GLN:CD	1.95	0.92
1:A:392:LYS:HD2	1:A:393:ASP:H	1.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:LEU:HG	3:A:1001:HOH:O	1.75	0.85
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:A:528:MET:HE3	1:A:574:ILE:HG21	1.67	0.76
1:B:538:LYS:CE	1:B:539:LYS:H	1.98	0.76
1:B:401:THR:HG22	1:B:401:THR:O	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:B:293:MET:HE3	1:B:315:TRP:HB2	1.71	0.72
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:377:ASN:C	1:B:377:ASN:HD22	1.99	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:B:651:ILE:HG21	1:B:755:MET:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:528:MET:HE2	1:A:530:LEU:HD21	1.73	0.69
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
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:630:SER:OG	1:B:740:HIS:NE2	2.27	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:A:500:LEU:CA	1:A:503:MET:HE3	2.23	0.67
1:B:203:TYR:HD2	1:B:207:VAL:HG21	1.57	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:651:ILE:CG2	1:B:755:MET:HE3	2.25	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: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:B:415:LEU:C	1:B:415:LEU:HD23	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:NZ	1:A:105:TYR:HB2	2.13	0.63
1:A:392:LYS:CD	1:A:393:ASP:H	2.08	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
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:B:627:TRP:CE3	1:B:755:MET:HE1	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:A:197:GLY:C	1:A:213:ALA:HB3	2.24	0.61
1:B:60:LEU:HD13	1:B:469:GLN:CD	2.26	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:205:GLU:OE2	2:B:767:U1N:H111	2.00	0.60
1:B:452:GLU:HG3	3:B:1004:HOH:O	2.01	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: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:HG12	1:B:295:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:HD2	3:A:933:HOH:O	2.01	0.59
1:B:272:ASN:C	1:B:272:ASN:HD22	2.10	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
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:HG2	1:B:358:ARG:HH11	1.68	0.58
1:A:111:GLY:O	1:A:137:LEU:HD12	2.04	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:N	1:B:445:LEU:HD22	2.19	0.57
1:B:520:ASN:O	1:B:521:GLU:HB3	2.03	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: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: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:H	1:A:143:ILE:HD12	1.71	0.56
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.35	0.56
1:A:205:GLU:OE2	2:A:767:U1N:H111	2.05	0.56
1:A:96:ASP:C	1:A:98:PHE:H	2.14	0.56
1:A:193:ILE:HG22	1:A:194:ILE:HG13	1.86	0.56
1:A:223:LEU:HB3	1:A:271:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:C	1:A:343:ARG:H	2.12	0.56
1:A:543:LEU:HD21	1:A:627:TRP:HD1	1.71	0.56
1:B:390:ASP:CG	1:B:390:ASP:O	2.48	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: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:B:72:GLN:C	1:B:74:ASN:H	2.15	0.55
1:A:155:VAL:HG22	1:A:166:TYR:HB2	1.87	0.55
1:A:289:ALA:CB	1:A:290:PRO:CA	2.79	0.55
1:B:765:LEU:HB3	1:B:766:PRO:C	2.31	0.55
1:B:78:VAL:HG12	1:B:87:SER:O	2.05	0.55
1:A:528:MET:HE1	1:A:618:PHE:CE1	2.42	0.55
1:A:741:GLY:O	1:A:742:ILE:C	2.48	0.55
1:B:293:MET:HE3	1:B:315:TRP:CB	2.36	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:HG2	1:B:358:ARG:NH1	2.21	0.54
1:B:741:GLY:O	1:B:742:ILE:C	2.50	0.54
1:A:39:SER:O	1:A:40:ARG:HB2	2.08	0.54
1:B:602:GLU:HG3	1:B:603:VAL:N	2.22	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: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:72:GLN:HB2	1:A:75:ASN:O	2.09	0.53
1:A:492:ARG:HG3	3:A:979:HOH:O	2.08	0.53
1:A:581:ARG:HG2	1:A:593:ALA:HB1	1.91	0.53
1:B:733:MET:HE3	1:B:734:TRP:O	2.08	0.53
1:A:40:ARG:HB3	1:A:506:ASN:O	2.07	0.53
1:A:289:ALA:HB1	1:A:290:PRO:C	2.34	0.53
1:A:658:ARG:HD3	1:A:660:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:SER:C	1:A:110:ASP:H	2.16	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
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:658:ARG:HG3	1:A:658:ARG:O	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:A:528:MET:CE	1:A:574:ILE:HG21	2.37	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:197:GLY:C	1:B:213:ALA:HB3	2.35	0.52
1:B:147:ARG:HB3	1:B:147:ARG:HH11	1.75	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:332:GLU:O	1:B:332:GLU:HG2	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:A:272:ASN:C	1:A:272:ASN:HD22	2.19	0.51
1:A:657:SER:OG	1:A:689:MET:HE1	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:60:LEU:HD13	1:B:469:GLN:OE1	2.11	0.51
1:B:401:THR:O	1:B:401:THR:CG2	2.57	0.51
1:A:597:ARG:HH12	1:A:679:ASN:HD21	1.57	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:A:215:TRP:CZ3	1:A:268:PHE:HE1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:98:PHE:CE1	1:B:100:HIS:HB2	2.46	0.50
1:B:289:ALA:HB3	3:B:964:HOH:O	2.11	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: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
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:51:ASN:ND2	1:B:54:ARG:HD3	2.25	0.50
1:B:64:SER:C	1:B:463:LYS:HB2	2.36	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:A:543:LEU:HD21	1:A:627:TRP:CD1	2.47	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:78:VAL:HG12	1:A:87:SER:O	2.11	0.49
1:A:486:VAL:CG1	1:A:487:ASN:N	2.76	0.49
1:A:95:PHE:CE1	1:A:116:LEU:HD11	2.48	0.49
1:A:718:GLN:HE21	1:A:718:GLN:HA	1.76	0.49
1:B:80:ASN:OD1	1:B:82:GLU:HB3	2.13	0.49
1:B:243:ASP:HB3	3:B:849:HOH:O	2.12	0.49
1:B:289:ALA:HB1	1:B:290:PRO:C	2.38	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:596:ARG:C	1:A:597:ARG:HD2	2.38	0.48
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:HD23	1:A:542:LEU:C	2.39	0.48
1:A:547:TYR:CD1	1:A:547:TYR:C	2.91	0.48
1:A:55:LEU:HD11	1:A:561:LEU:HD22	1.95	0.48
1:A:60:LEU:HD12	1:A:60:LEU:C	2.38	0.48
1:A:502:LYS:O	1:A:505:GLN:HG2	2.13	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
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:334:SER:OG	1:B:336:ARG:HG2	2.14	0.48
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.39	0.47
1:A:70:TYR:O	1:A:72:GLN:N	2.47	0.47
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:B:109:PRO:HG2	1:B:158:SER:O	2.14	0.47
1:B:515:ASP:CG	1:B:516:PHE:H	2.22	0.47
1:A:514:LEU:HD22	1:A:525:TRP:HE3	1.80	0.47
1:A:518:ILE:C	3:A:1001:HOH:O	2.58	0.47
1:B:124:TRP:HB2	1:B:204:GLU:OE2	2.14	0.47
1:B:293:MET:HE3	1:B:315:TRP:C	2.38	0.47
1:B:648:LYS:HE2	1:B:762:CYS:O	2.14	0.47
1:A:519:LEU:O	1:A:520:ASN:C	2.57	0.47
1:B:74:ASN:HB3	1:B:92:ASN:OD1	2.15	0.47
1:A:492:ARG:NH1	1:A:492:ARG:HG2	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:319:ILE:C	1:A:321:ASN:H	2.22	0.47
1:A:415:LEU:C	1:A:415:LEU:CD1	2.87	0.47
1:A:535:ASP:OD1	1:A:537:SER:HB3	2.14	0.47
1:B:208:PHE:O	1:B:209:SER:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:TRP:CZ3	1:B:755:MET:HE1	2.49	0.47
1:B:734:TRP:CD1	1:B:734:TRP:C	2.93	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:B:547:TYR:C	1:B:547:TYR:CD2	2.91	0.47
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.63	0.47
1:A:176:ILE:N	1:A:176:ILE:HD12	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: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:81:ALA:O	1:B:492:ARG:NH2	2.36	0.46
1:B:173:TYR:CZ	1:B:184:ARG:HG3	2.51	0.46
1:B:40:ARG:HG2	1:B:40:ARG:HH11	1.81	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: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:B:58:TYR:CD1	1:B:60:LEU:HD11	2.46	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:256:TYR:CD1	1:B:256:TYR:C	2.94	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:341:VAL:HG22	1:A:342:ALA:N	2.30	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:H	1:A:143:ILE:CD1	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:A:142:LEU:O	1:A:144:THR:HG23	2.16	0.45
1:A:244:GLU:CD	1:B:689:MET:HG3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PRO:HG3	1:A:326:ASP:OD2	2.17	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:76:ILE:HB	1:A:90:LEU:HD13	1.98	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: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:751:ILE:O	1:B:755:MET:HG3	2.16	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: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: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
1:A:492:ARG:HG2	1:A:492:ARG:HH11	1.82	0.44
1:B:538:LYS:HD3	1:B:539:LYS:N	2.32	0.44
1:A:242:SER:OG	1:A:243:ASP:N	2.48	0.44
1:B:289:ALA:CA	1:B:294:LEU:HD11	2.47	0.44
1:A:730:PHE:CZ	1:B:733:MET:HE1	2.53	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:60:LEU:HD12	1:A:60:LEU:O	2.17	0.44
1:A:145:GLU:CG	1:A:179:ASN:HB2	2.48	0.44
1:B:60:LEU:HD11	1:B:469:GLN:NE2	2.32	0.44
1:B:273:THR:HA	1:B:276:LEU:HG	2.00	0.44
1:A:108:SER:C	1:A:110:ASP:N	2.76	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:O	1:B:658:ARG:HG3	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: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:75:ASN:HB3	1:B:91:GLU:C	2.43	0.43
1:B:377:ASN:C	1:B:377:ASN:ND2	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:LYS:O	1:B:489:LYS:HG3	2.17	0.43
1:A:63:ILE:CG2	1:A:69:LEU:HG	2.49	0.43
1:A:93:SER:O	1:A:94:THR:C	2.61	0.43
1:A:295:ILE:CD1	1:A:317:ARG:HH21	2.31	0.43
1:A:612:GLN:HE21	1:A:612:GLN:HB3	1.53	0.43
1:B:385:CYS:SG	1:B:387:PHE:CE2	3.11	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: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:A:254:VAL:HA	1:A:255:PRO:HD3	1.91	0.43
1:A:489:LYS:NZ	3:A:1013:HOH:O	2.50	0.43
1:B:51:ASN:HD21	1:B:54:ARG:HG3	1.83	0.43
1:B:152:THR:HG21	1:B:155:VAL:HG22	2.00	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:458:SER:OG	1:A:471:ARG:HB2	2.19	0.43
1:A:546:VAL:HG22	1:A:547:TYR:N	2.34	0.43
1:B:74:ASN:O	1:B:92:ASN:HA	2.18	0.43
1:A:90:LEU:HD22	1:A:90:LEU:C	2.44	0.43
1:A:145:GLU:CD	1:A:179:ASN:HB2	2.44	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:256:TYR:CD1	1:A:256:TYR:C	2.97	0.42
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: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: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:215:TRP:CZ2	1:B:303:VAL:HG11	2.54	0.42
1:B:269:PHE:CE2	1:B:286:GLN:HG3	2.54	0.42
1:B:415:LEU:C	1:B:415:LEU:CD2	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:62:TRP:HB3	3:A:901:HOH:O	2.18	0.42
1:A:438:ASP:C	1:A:440:THR:H	2.28	0.42
1:A:607:ILE:HG22	1:A:611:ARG:NH1	2.34	0.42
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.55	0.42
1:A:382:ARG:HH21	1:A:591:MET:HE1	1.84	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:A:134:ILE:O	1:A:143:ILE:HD13	2.19	0.42
1:A:146:GLU:CD	1:A:181:PRO:HG3	2.45	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:B:761:GLN:C	1:B:761:GLN:OE1	2.62	0.42
1:A:535:ASP:CG	1:A:537:SER:HB3	2.45	0.42
1:A:691:ARG:HH11	1:A:691:ARG:HG3	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
1:A:41:LYS:NZ	1:A:47:ASP:OD2	2.52	0.42
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: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:47:ASP:HA	1:A:52:THR:CG2	2.49	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: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:136:ASP:CG	1:B:139:LYS:HG2	2.45	0.41
1:B:658:ARG:HD3	1:B:660:GLU:HB2	2.01	0.41
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.36	0.41
1:B:215:TRP:CE2	1:B:303:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:HG22	1:B:135:TYR:HB3	2.01	0.41
1:B:741:GLY:C	1:B:743:ALA:N	2.78	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:106:SER:HG	1:A:157:TRP:CD1	2.39	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:A:526:TYR:CD1	1:A:526:TYR:C	2.99	0.41
1:A:528:MET:HE2	1:A:530:LEU:CD2	2.45	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:69:LEU:HA	1:B:77:LEU:O	2.21	0.41
1:B:72:GLN:C	1:B:74:ASN:N	2.79	0.41
1:B:154:TRP:CE2	1:B:156:THR:HG23	2.56	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:538:LYS:HE3	1:B:539:LYS:N	2.32	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:341:VAL:C	1:A:343:ARG:N	2.77	0.41
1:B:751:ILE:HG23	1:B:752:TYR:N	2.35	0.41
1:B:60:LEU:N	1:B:60:LEU:HD12	2.36	0.40
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
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:B:761:GLN:C	1:B:761:GLN:CD	2.90	0.40
1:A:310:ARG:NH1	1:A:343:ARG:NH2	2.64	0.40
1:A:342:ALA:HA	3:A:873:HOH:O	2.21	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:A:666:TYR:CD1	1:A:666:TYR:C	2.99	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:415:LEU:HB2	1:A:436:LEU:HD11	2.03	0.40
1:A:677:GLU:H	1:A:677:GLU:CD	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:GLN:NE2	3:A:995:HOH:O	2.55	0.40
1:B:110:ASP:C	1:B:110:ASP:OD1	2.64	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:675:THR:C	1:A:680:LEU:HB2	2.47	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%)	11	8
1	B	726/728 (100%)	662 (91%)	56 (8%)	8 (1%)	11	8
All	All	1450/1456 (100%)	1323 (91%)	111 (8%)	16 (1%)	11	8

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

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Mol	Chain	Res	Type
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%)	603 (93%)	48 (7%)	13	10
1	B	653/653 (100%)	599 (92%)	54 (8%)	10	8
All	All	1304/1306 (100%)	1202 (92%)	102 (8%)	11	9

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	61	ARG
1	A	72	GLN
1	A	90	LEU
1	A	105	TYR
1	A	110	ASP
1	A	141	GLN
1	A	147	ARG
1	A	170	ASN
1	A	184	ARG
1	A	207	VAL
1	A	214	LEU
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	288	THR
1	A	303	VAL
1	A	313	LEU

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Mol	Chain	Res	Type
1	A	341	VAL
1	A	373	LYS
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	482	LEU
1	A	489	LYS
1	A	507	VAL
1	A	514	LEU
1	A	543	LEU
1	A	547	TYR
1	A	561	LEU
1	A	581	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	726	VAL
1	A	736	THR
1	A	761	GLN
1	B	54	ARG
1	B	75	ASN
1	B	90	LEU
1	B	125	ARG
1	B	129	THR
1	B	170	ASN
1	B	182	SER
1	B	184	ARG
1	B	223	LEU
1	B	232	GLU
1	B	236	ILE
1	B	246	LEU

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Mol	Chain	Res	Type
1	B	295	ILE
1	B	301	CYS
1	B	303	VAL
1	B	308	GLN
1	B	333	SER
1	B	338	ASN
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	418	ILE
1	B	429	ARG
1	B	436	LEU
1	B	445	LEU
1	B	452	GLU
1	B	486	VAL
1	B	489	LYS
1	B	502	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	597	ARG
1	B	598	LEU
1	B	608	GLU
1	B	612	GLN
1	B	673	LEU
1	B	689	MET
1	B	701	LEU
1	B	702	LEU
1	B	728	VAL
1	B	742	ILE
1	B	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	74	ASN
1	A	112	GLN
1	A	119	ASN
1	A	141	GLN
1	A	150	ASN
1	A	169	ASN
1	A	170	ASN
1	A	227	GLN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	338	ASN
1	A	344	GLN
1	A	483	HIS
1	A	487	ASN
1	A	505	GLN
1	A	508	GLN
1	A	572	ASN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	761	GLN
1	B	51	ASN
1	B	72	GLN
1	B	103	ASN
1	B	112	GLN
1	B	126	HIS
1	B	138	ASN
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	281	ASN
1	B	286	GLN
1	B	314	GLN
1	B	344	GLN
1	B	345	HIS
1	B	377	ASN
1	B	508	GLN

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Mol	Chain	Res	Type
1	B	572	ASN
1	B	595	ASN
1	B	612	GLN
1	B	685	ASN
1	B	694	ASN
1	B	710	ASN
1	B	712	HIS
1	B	718	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2.22	12 (48%)	32,33,33	1.70	7 (21%)
2	U1N	B	767	-	25,25,25	2.23	12 (48%)	32,33,33	1.66	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	-	-	5/18/18/18	0/2/2/2
2	U1N	B	767	-	-	3/18/18/18	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	767	U1N	C23-N24	5.49	1.43	1.33
2	A	767	U1N	C23-N24	5.16	1.42	1.33
2	B	767	U1N	C22-C16	3.34	1.44	1.39
2	A	767	U1N	C13-C14	3.22	1.55	1.51
2	B	767	U1N	C17-C16	3.11	1.44	1.39
2	A	767	U1N	C17-C16	3.05	1.44	1.39
2	B	767	U1N	C6-C1	3.02	1.44	1.39
2	A	767	U1N	C2-C1	2.96	1.43	1.39
2	A	767	U1N	C22-C16	2.90	1.43	1.39
2	B	767	U1N	C18-C17	2.81	1.43	1.38
2	A	767	U1N	C6-C1	2.65	1.43	1.39
2	A	767	U1N	C16-C14	2.56	1.53	1.49
2	B	767	U1N	C21-C19	2.49	1.42	1.37
2	B	767	U1N	C2-C1	2.46	1.43	1.39
2	A	767	U1N	C3-C2	2.44	1.42	1.38
2	A	767	U1N	C21-C19	2.39	1.41	1.37
2	B	767	U1N	C1-C23	-2.38	1.47	1.50
2	A	767	U1N	C18-C19	2.34	1.41	1.37
2	B	767	U1N	C18-C19	2.28	1.41	1.37
2	A	767	U1N	C3-C4	2.26	1.43	1.38
2	B	767	U1N	C6-C5	2.22	1.42	1.38
2	B	767	U1N	C3-C2	2.20	1.42	1.38
2	B	767	U1N	C22-C21	2.16	1.42	1.38
2	A	767	U1N	C18-C17	2.09	1.42	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	767	U1N	O25-C23-N24	-4.82	115.65	122.62
2	B	767	U1N	O25-C23-N24	-4.66	115.88	122.62
2	A	767	U1N	O15-C14-C13	3.71	123.14	119.96
2	B	767	U1N	O15-C14-C13	3.18	122.69	119.96
2	A	767	U1N	O15-C14-C16	-3.08	116.61	120.73
2	B	767	U1N	O25-C23-C1	3.03	123.30	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	767	U1N	O25-C23-C1	2.98	123.24	119.60
2	B	767	U1N	O15-C14-C16	-2.89	116.86	120.73
2	A	767	U1N	C1-C23-N24	2.74	121.11	117.74
2	B	767	U1N	C11-C9-C8	-2.66	106.64	111.48
2	A	767	U1N	C11-C9-C8	-2.51	106.91	111.48
2	B	767	U1N	C1-C23-N24	2.49	120.81	117.74
2	B	767	U1N	C13-C14-C16	2.33	120.45	118.51
2	A	767	U1N	C13-C14-C16	2.09	120.24	118.51

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

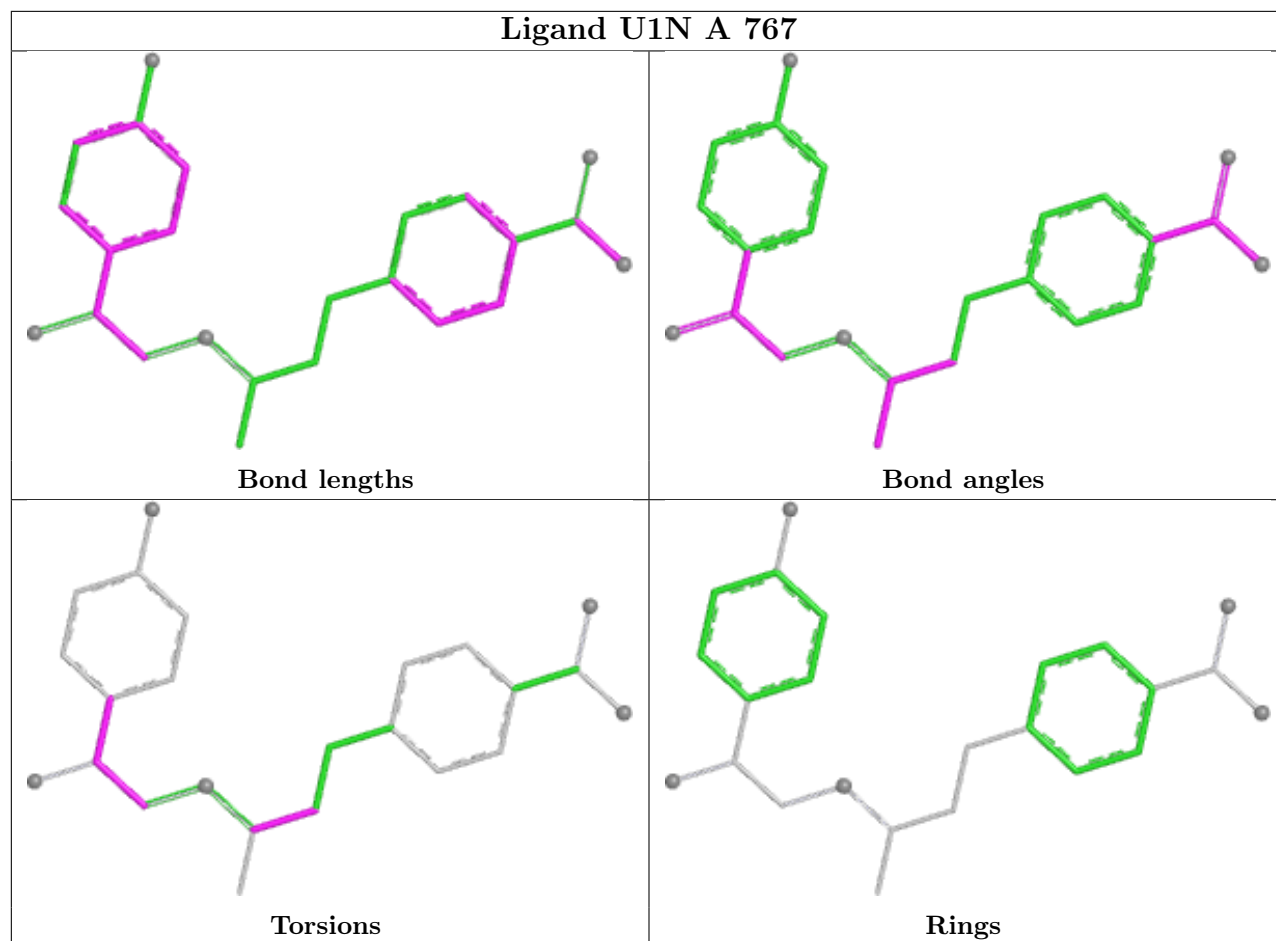
There are no ring outliers.

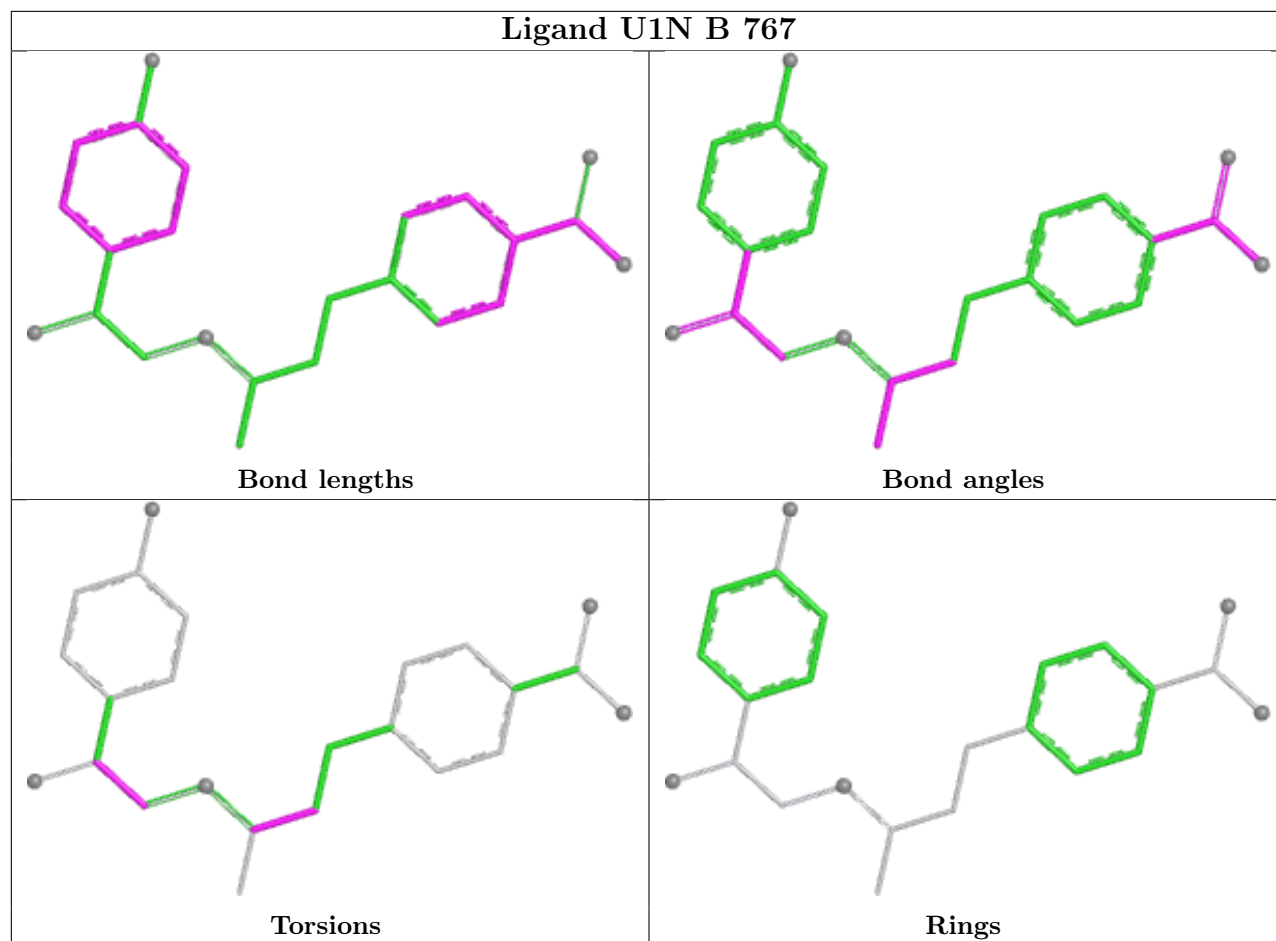
2 monomers are involved in 2 short contacts:

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.

Ligand U1N A 767





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%)	0.58	83 (11%) 10 10	17, 31, 70, 93	0
1	B	728/728 (100%)	0.56	70 (9%) 13 14	18, 31, 62, 87	0
All	All	1454/1456 (99%)	0.57	153 (10%) 11 12	17, 31, 66, 93	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	11.1
1	B	39	SER	7.9
1	A	39	SER	7.1
1	B	765	LEU	6.3
1	A	90	LEU	5.5
1	A	71	LYS	5.4
1	B	766	PRO	5.2
1	B	40	ARG	5.1
1	A	83	TYR	5.0
1	A	105	TYR	4.8
1	A	342	ALA	4.8
1	B	74	ASN	4.7
1	A	279	VAL	4.6
1	A	289	ALA	4.6
1	A	70	TYR	4.5
1	A	79	PHE	4.4
1	A	76	ILE	4.4
1	B	521	GLU	4.4
1	A	138	ASN	4.3
1	B	76	ILE	4.3
1	B	71	LYS	4.3
1	A	95	PHE	4.2
1	B	278	SER	4.1
1	A	98	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	114	ILE	4.1
1	A	139	LYS	4.1
1	B	81	ALA	4.0
1	B	72	GLN	4.0
1	A	78	VAL	4.0
1	B	83	TYR	4.0
1	B	73	GLU	3.9
1	A	77	LEU	3.9
1	A	160	VAL	3.8
1	A	392	LYS	3.8
1	B	338	ASN	3.8
1	B	289	ALA	3.7
1	B	385	CYS	3.7
1	A	84	GLY	3.6
1	A	103	ASN	3.6
1	B	82	GLU	3.6
1	B	95	PHE	3.6
1	A	94	THR	3.5
1	B	452	GLU	3.5
1	B	77	LEU	3.5
1	B	277	SER	3.4
1	A	74	ASN	3.4
1	B	138	ASN	3.4
1	B	88	VAL	3.4
1	A	87	SER	3.4
1	A	40	ARG	3.3
1	B	399	LYS	3.3
1	A	102	ILE	3.3
1	A	506	ASN	3.3
1	A	100	HIS	3.2
1	B	301	CYS	3.2
1	A	72	GLN	3.1
1	B	78	VAL	3.1
1	A	137	LEU	3.1
1	A	89	PHE	3.1
1	A	81	ALA	3.1
1	A	134	ILE	3.1
1	B	86	SER	3.1
1	B	280	THR	3.1
1	B	84	GLY	3.0
1	B	439	TYR	3.0
1	B	471	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	70	TYR	3.0
1	A	333	SER	2.9
1	B	621	ASN	2.9
1	A	334	SER	2.9
1	A	276	LEU	2.9
1	B	90	LEU	2.9
1	B	761	GLN	2.9
1	B	87	SER	2.9
1	A	538	LYS	2.9
1	B	98	PHE	2.9
1	A	142	LEU	2.8
1	B	92	ASN	2.8
1	B	100	HIS	2.8
1	B	99	GLY	2.8
1	B	283	THR	2.8
1	B	85	ASN	2.8
1	B	219	ASN	2.8
1	A	505	GLN	2.8
1	B	276	LEU	2.8
1	A	75	ASN	2.7
1	A	179	ASN	2.7
1	A	110	ASP	2.7
1	B	97	GLU	2.7
1	A	450	ASN	2.7
1	A	341	VAL	2.7
1	A	379	GLU	2.6
1	B	89	PHE	2.6
1	A	69	LEU	2.6
1	A	502	LYS	2.6
1	A	513	LYS	2.6
1	A	336	ARG	2.6
1	B	60	LEU	2.6
1	A	145	GLU	2.6
1	B	75	ASN	2.6
1	B	61	ARG	2.6
1	B	140	ARG	2.6
1	A	278	SER	2.6
1	A	321	ASN	2.5
1	B	334	SER	2.5
1	A	180	LEU	2.5
1	B	91	GLU	2.5
1	B	102	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	135	TYR	2.5
1	B	413	ASP	2.5
1	A	82	GLU	2.5
1	A	99	GLY	2.5
1	A	61	ARG	2.5
1	B	506	ASN	2.5
1	A	96	ASP	2.5
1	B	391	LYS	2.5
1	A	80	ASN	2.5
1	A	176	ILE	2.5
1	A	183	TYR	2.4
1	A	507	VAL	2.4
1	A	764	SER	2.4
1	A	452	GLU	2.4
1	A	393	ASP	2.4
1	B	295	ILE	2.4
1	A	615	LYS	2.4
1	A	85	ASN	2.3
1	A	115	LEU	2.3
1	A	377	ASN	2.3
1	A	141	GLN	2.2
1	B	101	SER	2.2
1	A	253	ARG	2.2
1	A	73	GLU	2.2
1	A	144	THR	2.2
1	A	88	VAL	2.2
1	A	489	LYS	2.2
1	B	80	ASN	2.2
1	B	207	VAL	2.2
1	B	141	GLN	2.2
1	B	93	SER	2.2
1	A	487	ASN	2.2
1	B	520	ASN	2.2
1	B	187	TRP	2.2
1	A	136	ASP	2.2
1	A	143	ILE	2.1
1	A	92	ASN	2.1
1	A	697	GLN	2.1
1	B	743	ALA	2.1
1	A	280	THR	2.1
1	B	523	LYS	2.1
1	B	51	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	79	PHE	2.1
1	A	209	SER	2.1
1	B	41	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

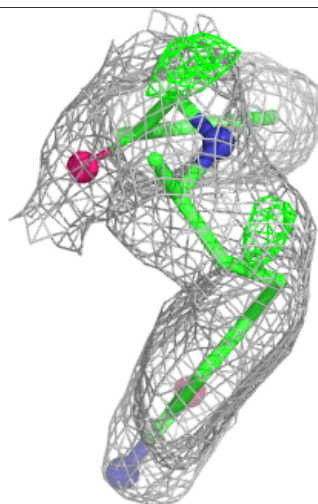
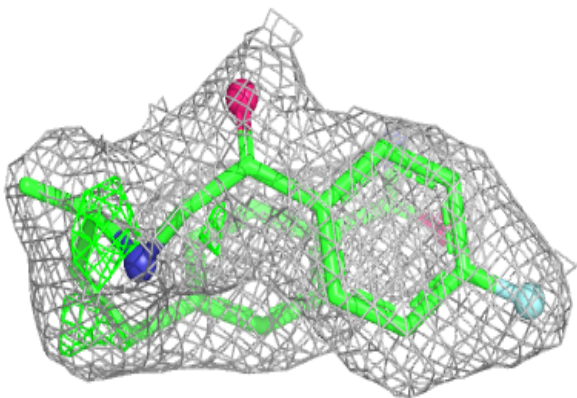
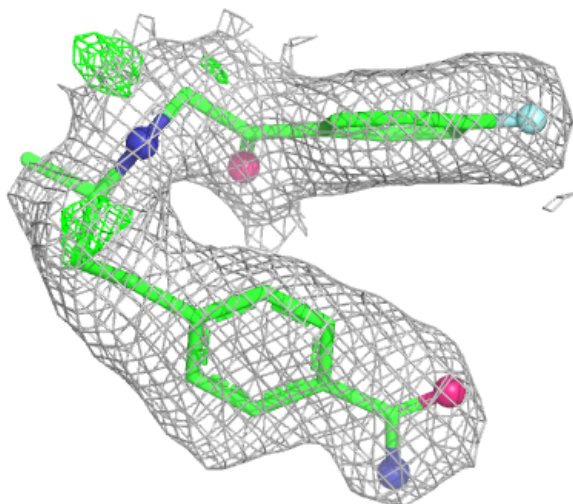
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	U1N	A	767	24/24	0.87	0.15	36,46,50,53	0
2	U1N	B	767	24/24	0.90	0.17	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.

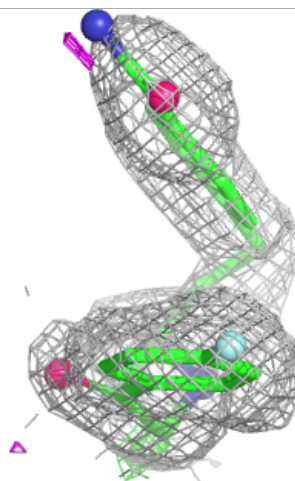
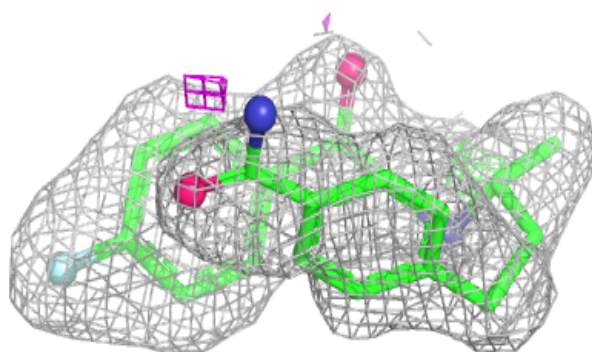
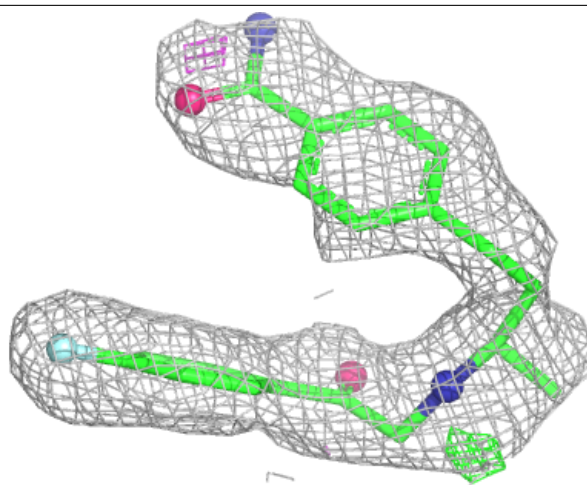
Electron density around U1N A 767:

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



Electron density around U1N B 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.