



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:17 PM UTC

PDB ID : 3UKU / pdb_00003uku
Title : Structure of Arp2/3 complex with bound inhibitor CK-869
Authors : Nolen, B.J.; Han, M.
Deposited on : 2011-11-09
Resolution : 2.75 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

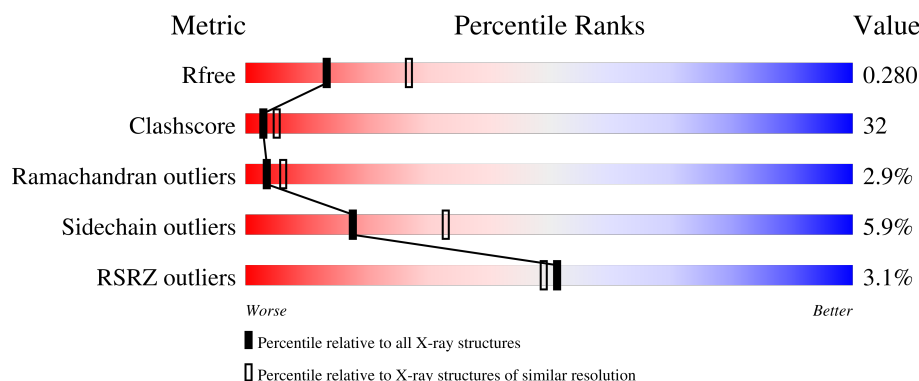
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	418	
2	B	394	
3	C	372	
4	D	300	
5	E	178	

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Mol	Chain	Length	Quality of chain
6	F	168	 % 48% 44% 7% ..
7	G	151	 11% 54% 36% • 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	C69	A	501	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13460 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 ACTIN-LIKE PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3197	2053	534	595	15			

- Molecule 2 is a protein called ACTIN-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1528	979	261	284	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	341	Total	C	N	O	S	0	0	0
			2633	1669	460	485	19			

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	277	Total	C	N	O	S	0	0	0
			2217	1410	381	418	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	173	Total	C	N	O	S	0	0	0
			1403	901	234	259	9			

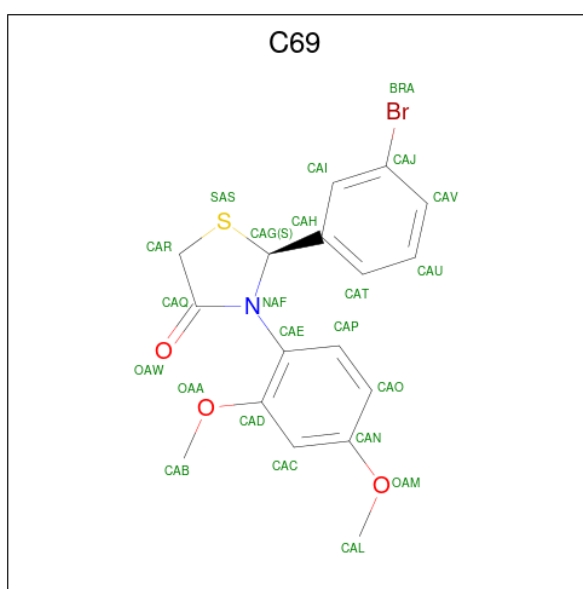
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	166	Total	C	N	O	S	0	0	0
			1364	871	238	246	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	138	Total	C	N	O	S	0	0	0
			971	609	171	190	1			

- Molecule 8 is (2S)-2-(3-bromophenyl)-3-(2,4-dimethoxyphenyl)-1,3-thiazolidin-4-one (CCD ID: C69) (formula: C₁₇H₁₆BrNO₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	Br	C	N	O	S	0	0
			23	1	17	1	3	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	25	Total	O	0	0
			25	25		
9	B	11	Total	O	0	0
			11	11		
9	C	37	Total	O	0	0
			37	37		
9	D	26	Total	O	0	0
			26	26		

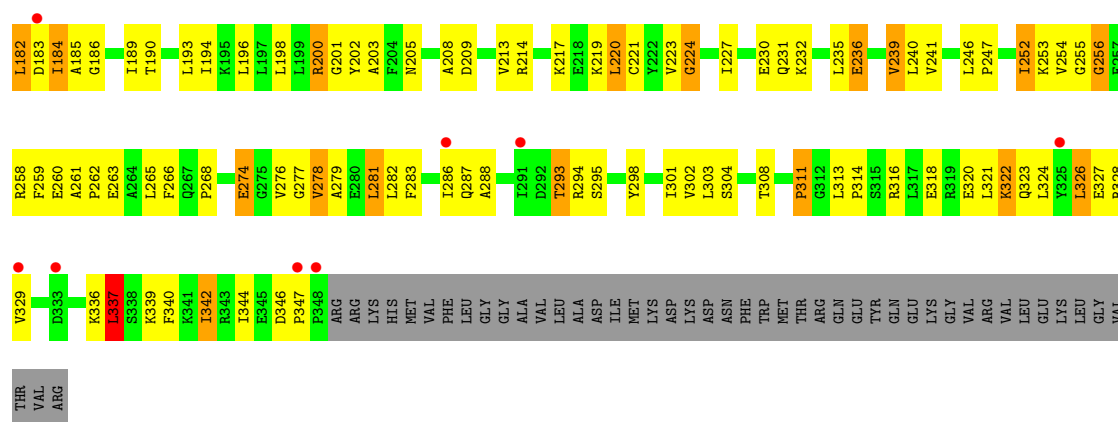
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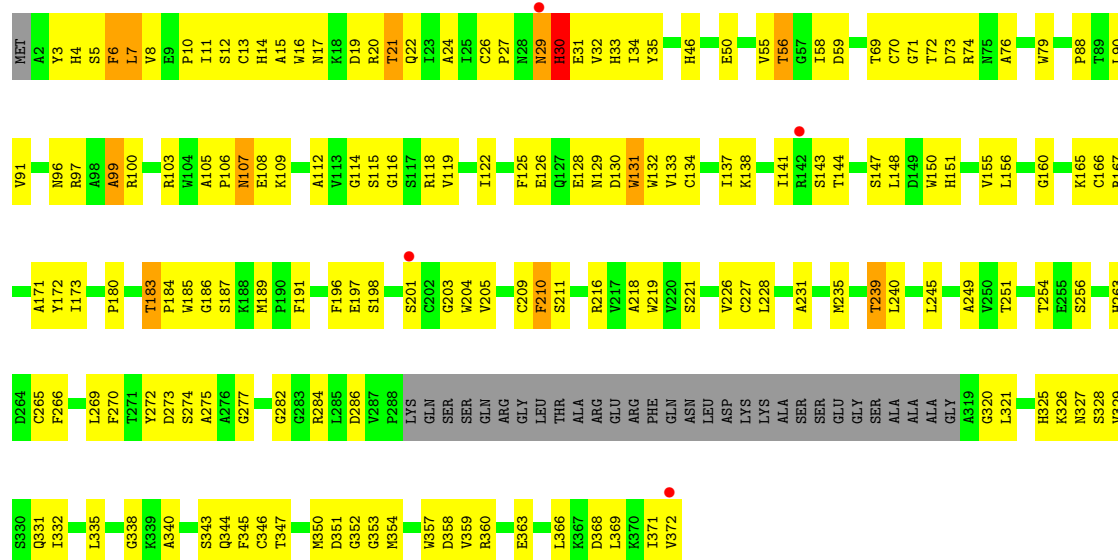
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	6	Total 6	O 6	0	0
9	F	15	Total 15	O 15	0	0
9	G	4	Total 4	O 4	0	0

- Molecule 1: ACTIN-LIKE PROTEIN 3

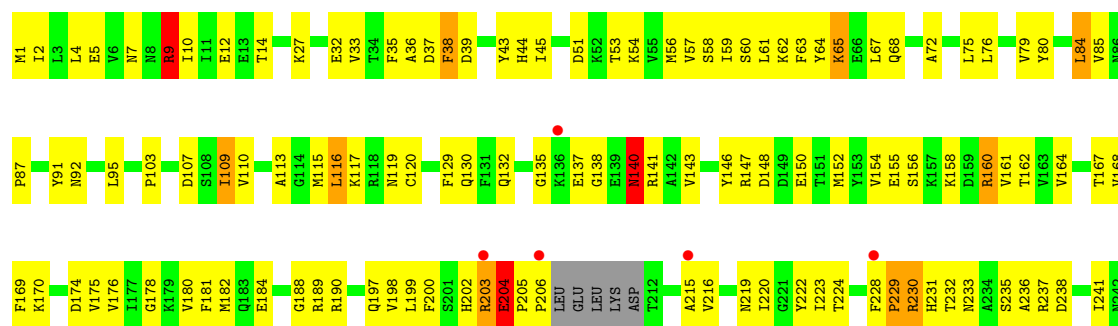
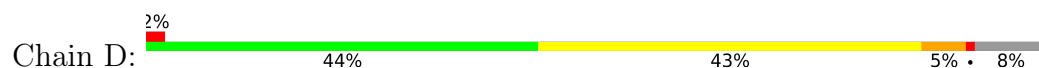


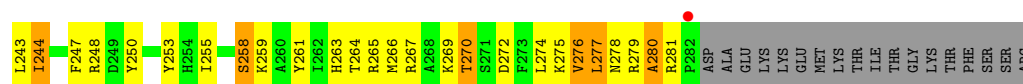


• Molecule 3: Actin-related protein 2/3 complex subunit 1B

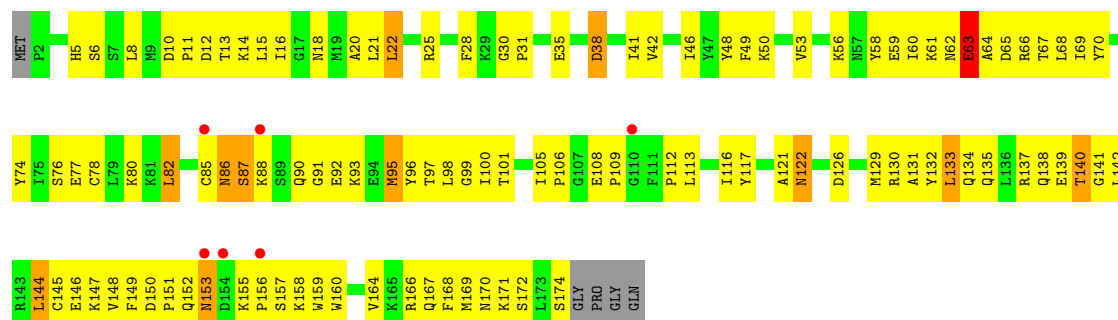


• Molecule 4: Actin-related protein 2/3 complex subunit 2

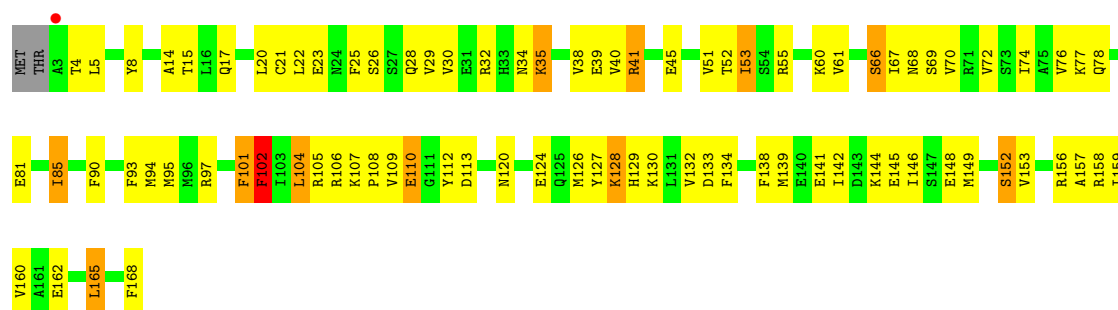




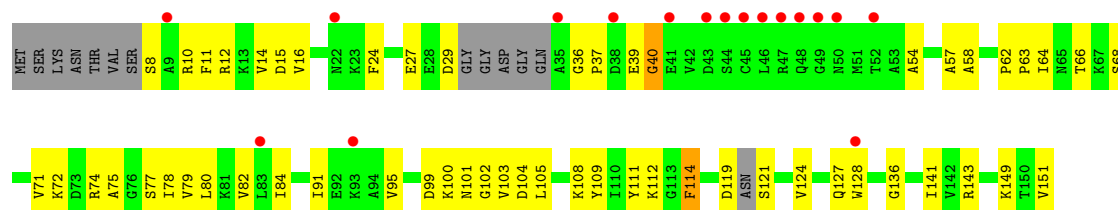
• Molecule 5: Actin-related protein 2/3 complex subunit 3



• Molecule 6: Actin-related protein 2/3 complex subunit 4



• Molecule 7: Actin-related protein 2/3 complex subunit 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.11Å 129.66Å 203.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.75) 91.1 (20.00-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.301 0.238 , 0.280	Depositor DCC
R_{free} test set	3873 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13460	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: C69

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	0.52	0/3278	1.08	24/4447 (0.5%)
2	B	0.49	0/1557	0.99	7/2110 (0.3%)
3	C	0.56	0/2702	1.05	13/3673 (0.4%)
4	D	0.50	0/2265	1.03	13/3062 (0.4%)
5	E	0.39	0/1437	0.97	4/1940 (0.2%)
6	F	0.57	0/1386	1.04	9/1858 (0.5%)
7	G	0.41	0/982	0.90	2/1330 (0.2%)
All	All	0.51	0/13607	1.03	72/18420 (0.4%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	160	TRP	N-CA-C	-8.64	104.77	114.62
4	D	204	GLU	CA-C-N	8.39	125.78	119.66
4	D	204	GLU	C-N-CA	8.39	125.78	119.66
1	A	178	ILE	N-CA-C	7.89	117.00	107.61
1	A	373	GLN	N-CA-C	7.58	119.18	111.07
3	C	72	THR	N-CA-C	-7.58	104.06	113.38
5	E	63	GLU	N-CA-C	-7.54	103.34	112.54
1	A	79	ARG	N-CA-C	6.92	120.45	108.76
4	D	280	ALA	N-CA-C	-6.85	104.73	113.23
4	D	79	VAL	N-CA-C	6.81	116.94	110.53
5	E	86	ASN	N-CA-C	6.71	119.00	110.61
1	A	327	MET	N-CA-C	6.70	118.66	111.36
3	C	30	HIS	N-CA-C	-6.63	105.16	112.72
3	C	11	ILE	N-CA-C	-6.41	98.63	107.99
1	A	31	ILE	N-CA-C	6.39	116.12	108.45
6	F	102	PHE	N-CA-C	6.37	124.37	110.80
1	A	404	GLY	CA-C-N	6.37	127.80	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	GLY	C-N-CA	6.37	127.80	119.84
7	G	112	LYS	N-CA-C	-6.22	103.81	112.45
3	C	245	LEU	CA-C-N	6.18	126.20	119.89
3	C	245	LEU	C-N-CA	6.18	126.20	119.89
6	F	148	GLU	N-CA-C	-6.14	104.51	111.14
3	C	165	LYS	N-CA-C	6.12	119.44	109.59
4	D	39	ASP	N-CA-C	6.04	119.89	111.74
3	C	147	SER	N-CA-C	5.99	119.30	109.72
1	A	320	VAL	N-CA-C	5.97	116.41	107.51
2	B	224	GLY	N-CA-C	-5.97	104.89	112.54
4	D	109	ILE	N-CA-C	-5.93	104.54	111.00
3	C	99	ALA	N-CA-C	-5.92	101.52	110.28
1	A	368	ILE	N-CA-C	5.86	116.54	107.99
6	F	30	VAL	N-CA-C	5.84	116.42	107.77
6	F	41	ARG	N-CA-C	5.83	119.71	112.24
1	A	134	PHE	N-CA-C	5.80	120.43	113.23
6	F	35	LYS	N-CA-C	5.79	115.58	108.11
1	A	252	TRP	N-CA-C	5.76	120.32	113.12
1	A	351	GLU	N-CA-C	-5.71	106.44	113.41
1	A	76	TRP	CA-C-N	5.69	126.96	119.84
1	A	76	TRP	C-N-CA	5.69	126.96	119.84
1	A	396	THR	N-CA-C	5.67	118.73	110.17
6	F	32	ARG	N-CA-C	5.65	119.36	111.74
1	A	72	TYR	N-CA-C	5.64	118.41	109.50
6	F	5	LEU	N-CA-C	5.63	118.62	111.69
1	A	326	THR	N-CA-C	-5.58	106.52	113.38
3	C	29	ASN	N-CA-CB	-5.56	101.99	110.49
4	D	27	LYS	CA-C-N	5.55	126.77	119.84
4	D	27	LYS	C-N-CA	5.55	126.77	119.84
1	A	16	TYR	N-CA-C	5.50	118.06	108.76
5	E	140	THR	N-CA-C	-5.49	105.69	112.38
4	D	276	VAL	N-CA-C	-5.47	104.54	110.23
6	F	101	PHE	N-CA-C	-5.42	99.25	110.80
3	C	239	THR	N-CA-C	5.37	118.21	109.24
4	D	107	ASP	N-CA-C	5.36	119.31	112.34
2	B	239	VAL	N-CA-C	5.35	118.56	111.17
4	D	36	ALA	N-CA-C	5.35	115.35	108.34
3	C	115	SER	N-CA-C	5.31	115.55	108.38
6	F	29	VAL	N-CA-C	5.30	118.54	111.44
1	A	126	THR	N-CA-C	-5.26	104.60	111.02
2	B	236	GLU	N-CA-C	5.24	119.52	113.18
1	A	26	GLU	CA-C-N	5.24	125.40	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	GLU	C-N-CA	5.24	125.40	119.90
1	A	109	TYR	N-CA-C	-5.18	103.56	110.55
7	G	141	ILE	N-CA-C	-5.18	105.35	111.00
2	B	293	THR	N-CA-C	-5.17	105.65	112.94
3	C	6	PHE	N-CA-C	-5.15	107.16	113.50
4	D	9	ARG	N-CA-C	5.15	121.76	110.80
2	B	214	ARG	N-CA-C	-5.13	105.58	111.07
4	D	162	THR	N-CA-C	5.13	117.26	108.90
2	B	337	LEU	N-CA-C	-5.12	105.78	112.23
2	B	328	ARG	N-CA-C	5.09	119.36	113.20
1	A	157	GLN	N-CA-C	-5.08	107.13	113.38
1	A	407	ILE	N-CA-C	5.06	115.67	110.36
3	C	137	ILE	N-CA-C	-5.03	100.01	107.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3197	0	3145	204	0
2	B	1528	0	1530	116	0
3	C	2633	0	2560	165	0
4	D	2217	0	2158	160	0
5	E	1403	0	1398	119	0
6	F	1364	0	1403	103	0
7	G	971	0	895	57	0
8	A	23	0	16	11	0
9	A	25	0	0	2	0
9	B	11	0	0	0	0
9	C	37	0	0	1	0
9	D	26	0	0	0	0
9	E	6	0	0	0	0
9	F	15	0	0	0	0
9	G	4	0	0	0	0
All	All	13460	0	13105	850	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 32.

All (850) 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)
2:B:182:LEU:HD11	2:B:278:VAL:H	1.12	1.12
3:C:183:THR:HG22	3:C:185:TRP:H	1.19	1.07
4:D:197:GLN:HE21	4:D:199:LEU:HD11	1.14	1.07
6:F:4:THR:HG23	6:F:55:ARG:HE	1.25	1.01
1:A:112:LEU:HD11	1:A:130:MET:HE2	1.41	0.97
5:E:167:GLN:HE21	5:E:172:SER:HB2	1.29	0.97
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.44	0.97
3:C:74:ARG:HG2	3:C:97:ARG:O	1.66	0.96
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.47	0.96
1:A:327:MET:HE2	1:A:374:ARG:HB2	1.45	0.95
2:B:163:VAL:HA	2:B:185:ALA:HB2	1.48	0.95
3:C:107:ASN:ND2	3:C:109:LYS:H	1.65	0.95
3:C:17:ASN:HD21	3:C:21:THR:HG22	1.30	0.94
1:A:126:THR:OG1	8:A:501:C69:H10	1.70	0.92
4:D:197:GLN:NE2	4:D:199:LEU:HD11	1.86	0.90
1:A:363:ILE:HD13	1:A:363:ILE:H	1.35	0.89
2:B:322:LYS:HB3	7:G:16:VAL:HG11	1.54	0.89
1:A:343:VAL:HG23	1:A:346:ARG:HH21	1.38	0.88
5:E:31:PRO:HG2	5:E:132:TYR:HB2	1.56	0.87
5:E:15:LEU:HD23	5:E:20:ALA:HA	1.55	0.86
5:E:95:MET:HG2	5:E:141:GLY:O	1.76	0.86
5:E:25:ARG:HG3	5:E:35:GLU:HB3	1.57	0.85
7:G:78:ILE:O	7:G:82:VAL:HG23	1.75	0.85
3:C:263:HIS:CD2	6:F:21:CYS:HB3	2.10	0.85
7:G:79:VAL:HG21	7:G:109:TYR:CE1	2.13	0.84
1:A:19:LEU:HD13	1:A:96:VAL:HG13	1.60	0.84
4:D:281:ARG:NH1	6:F:126:MET:HE2	1.93	0.83
2:B:182:LEU:HD11	2:B:278:VAL:N	1.92	0.83
1:A:206:GLN:HE21	5:E:166:ARG:HH22	1.27	0.82
3:C:96:ASN:O	3:C:97:ARG:HD3	1.78	0.82
2:B:279:ALA:HB1	2:B:320:GLU:HG2	1.60	0.81
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.61	0.80
3:C:32:VAL:HG22	3:C:58:ILE:HD11	1.64	0.80
3:C:254:THR:HA	3:C:340:ALA:O	1.80	0.80
1:A:206:GLN:HE21	5:E:166:ARG:NH2	1.81	0.79
3:C:107:ASN:C	3:C:107:ASN:HD22	1.88	0.79
3:C:183:THR:HB	3:C:189:MET:HE1	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:168:VAL:HG22	4:D:220:ILE:HG12	1.62	0.79
1:A:52:MET:HE2	1:A:56:ASP:HB3	1.65	0.79
4:D:140:ASN:HD22	4:D:140:ASN:N	1.79	0.79
2:B:236:GLU:HB3	6:F:105:ARG:HH12	1.49	0.78
2:B:279:ALA:CB	2:B:320:GLU:HG2	2.13	0.78
3:C:34:ILE:HB	3:C:46:HIS:HB2	1.66	0.78
2:B:346:ASP:HB3	3:C:74:ARG:HH22	1.49	0.77
6:F:25:PHE:CD1	6:F:67:ILE:HD13	2.20	0.77
3:C:10:PRO:HG2	6:F:124:GLU:HG2	1.66	0.77
4:D:33:VAL:HG12	4:D:35:PHE:HD2	1.48	0.76
3:C:14:HIS:H	3:C:331:GLN:HE22	1.32	0.75
1:A:155:SER:HB2	1:A:370:HIS:HB3	1.69	0.75
2:B:182:LEU:HG	2:B:281:LEU:HD12	1.69	0.75
5:E:100:ILE:HA	5:E:134:GLN:HE21	1.52	0.75
1:A:111:LEU:HD23	1:A:111:LEU:C	2.12	0.74
1:A:228:LYS:HA	1:A:232:SER:OG	1.87	0.74
1:A:343:VAL:CG2	1:A:363:ILE:HG13	2.18	0.74
1:A:223:THR:O	1:A:227:VAL:HG23	1.88	0.74
3:C:58:ILE:HG12	3:C:69:THR:HG22	1.69	0.74
6:F:146:ILE:HA	6:F:149:MET:HE2	1.70	0.74
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.70	0.73
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.70	0.73
4:D:189:ARG:CZ	4:D:197:GLN:HG3	2.19	0.73
8:A:501:C69:H12	8:A:501:C69:OAA	1.86	0.73
4:D:150:GLU:HG2	4:D:167:THR:HA	1.69	0.73
6:F:95:MET:HE1	6:F:108:PRO:HG3	1.70	0.73
4:D:64:TYR:CB	4:D:92:ASN:ND2	2.53	0.72
5:E:167:GLN:NE2	5:E:172:SER:HB2	2.03	0.72
1:A:239:VAL:HG11	5:E:48:TYR:HD1	1.54	0.72
6:F:4:THR:HG23	6:F:55:ARG:NE	2.04	0.72
2:B:274:GLU:OE1	2:B:274:GLU:HA	1.89	0.72
5:E:152:GLN:HB3	5:E:155:LYS:HZ1	1.54	0.72
3:C:325:HIS:HE1	3:C:353:GLY:O	1.73	0.72
3:C:284:ARG:HD3	3:C:286:ASP:O	1.90	0.71
5:E:113:LEU:HD22	5:E:116:ILE:HD12	1.72	0.71
1:A:33:SER:HB3	1:A:78:ILE:HD12	1.73	0.71
4:D:9:ARG:HG2	4:D:9:ARG:HH11	1.55	0.71
2:B:219:LYS:HG2	2:B:220:LEU:CD1	2.20	0.71
3:C:343:SER:O	3:C:359:VAL:HG23	1.91	0.71
7:G:80:LEU:O	7:G:84:ILE:HD13	1.89	0.71
1:A:18:LYS:N	1:A:18:LYS:HD3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:34:ASN:O	6:F:35:LYS:HG2	1.90	0.71
4:D:184:GLU:OE1	6:F:158:ARG:HB2	1.91	0.70
3:C:183:THR:HG22	3:C:185:TRP:N	2.00	0.70
6:F:77:LYS:O	6:F:78:GLN:HG3	1.91	0.70
5:E:38:ASP:OD2	5:E:38:ASP:N	2.23	0.70
1:A:97:ILE:HG22	1:A:98:PHE:CD2	2.27	0.70
3:C:27:PRO:HG3	3:C:33:HIS:CD2	2.27	0.70
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.73	0.70
4:D:197:GLN:HE21	4:D:199:LEU:CD1	2.00	0.70
4:D:45:ILE:HG12	4:D:57:VAL:HG22	1.73	0.70
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.27	0.70
5:E:77:GLU:HA	5:E:80:LYS:HD2	1.72	0.70
6:F:53:ILE:N	6:F:53:ILE:HD12	2.07	0.70
7:G:77:SER:HA	7:G:80:LEU:HB3	1.73	0.69
1:A:55:VAL:CG1	1:A:58:LEU:HD12	2.22	0.69
1:A:313:ARG:HB2	1:A:314:PRO:HD3	1.74	0.69
7:G:121:SER:O	7:G:124:VAL:HG12	1.90	0.69
1:A:19:LEU:HD23	1:A:19:LEU:N	2.07	0.69
1:A:98:PHE:CD1	4:D:253:TYR:HD1	2.11	0.69
4:D:33:VAL:HG12	4:D:35:PHE:CD2	2.27	0.69
4:D:64:TYR:HB3	4:D:92:ASN:ND2	2.07	0.69
4:D:205:PRO:HB3	4:D:222:TYR:CE2	2.27	0.69
1:A:91:ARG:HA	1:A:94:GLU:OE2	1.92	0.69
6:F:4:THR:CG2	6:F:55:ARG:HE	2.05	0.69
2:B:278:VAL:HG13	2:B:279:ALA:N	2.08	0.69
2:B:165:HIS:CD2	2:B:181:ARG:HG2	2.28	0.68
3:C:240:LEU:HD23	3:C:270:PHE:CE2	2.28	0.68
4:D:7:ASN:ND2	4:D:12:GLU:OE1	2.25	0.68
5:E:121:ALA:O	5:E:122:ASN:HB3	1.91	0.68
1:A:352:GLU:O	1:A:353:LEU:HD22	1.94	0.68
2:B:182:LEU:CD1	2:B:278:VAL:H	2.00	0.68
1:A:246:ASP:OD1	5:E:50:LYS:HE3	1.94	0.68
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.09	0.68
3:C:185:TRP:CZ3	3:C:235:MET:HG2	2.29	0.68
4:D:140:ASN:HD22	4:D:140:ASN:H	1.40	0.68
5:E:86:ASN:O	5:E:87:SER:HB3	1.93	0.68
1:A:409:ARG:HD3	2:B:200:ARG:O	1.94	0.67
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.76	0.67
4:D:188:GLY:HA3	6:F:165:LEU:HD23	1.75	0.67
2:B:175:LEU:HD23	2:B:175:LEU:N	2.10	0.67
4:D:59:ILE:O	4:D:91:TYR:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.29	0.67
1:A:369:THR:HA	1:A:373:GLN:OE1	1.95	0.67
3:C:107:ASN:HD22	3:C:108:GLU:N	1.93	0.67
3:C:107:ASN:HD22	3:C:109:LYS:H	1.41	0.66
5:E:65:ASP:O	5:E:69:ILE:HG13	1.94	0.66
6:F:38:VAL:HB	6:F:66:SER:HB3	1.77	0.66
6:F:128:LYS:O	6:F:132:VAL:HG23	1.94	0.66
2:B:193:LEU:HD23	2:B:213:VAL:HG12	1.76	0.66
1:A:363:ILE:H	1:A:363:ILE:CD1	2.08	0.66
2:B:282:LEU:HD23	2:B:321:LEU:HD11	1.77	0.66
3:C:185:TRP:HZ3	3:C:235:MET:HG2	1.59	0.66
3:C:201:SER:HB3	7:G:149:LYS:NZ	2.11	0.66
1:A:329:ARG:O	1:A:330:ASP:HB2	1.94	0.66
3:C:10:PRO:HB3	3:C:350:MET:HA	1.76	0.66
3:C:186:GLY:O	3:C:189:MET:HE3	1.95	0.66
1:A:343:VAL:HG21	1:A:363:ILE:HG13	1.77	0.66
1:A:84:GLU:HB3	8:A:501:C69:H7	1.77	0.65
5:E:42:VAL:HG13	5:E:140:THR:OG1	1.96	0.65
4:D:164:VAL:HG22	4:D:224:THR:HG23	1.78	0.65
6:F:8:TYR:CD1	6:F:55:ARG:HB2	2.32	0.65
1:A:163:LEU:HG	1:A:416:VAL:HG13	1.78	0.65
4:D:182:MET:HG3	4:D:200:PHE:CE1	2.32	0.65
1:A:28:GLN:HG2	4:D:10:ILE:HD13	1.79	0.65
2:B:193:LEU:HD23	2:B:213:VAL:CG1	2.26	0.65
1:A:55:VAL:HG12	1:A:55:VAL:O	1.98	0.64
3:C:116:GLY:C	3:C:118:ARG:H	2.03	0.64
3:C:151:HIS:HB2	3:C:210:PHE:CE1	2.32	0.64
8:A:501:C69:H9	8:A:501:C69:OAW	1.96	0.64
3:C:14:HIS:H	3:C:331:GLN:NE2	1.94	0.64
1:A:206:GLN:NE2	5:E:166:ARG:HH22	1.94	0.64
4:D:65:LYS:HB3	4:D:65:LYS:HZ2	1.62	0.64
4:D:160:ARG:HB3	4:D:160:ARG:HH11	1.63	0.64
2:B:227:ILE:HD11	2:B:263:GLU:OE2	1.97	0.64
1:A:343:VAL:HG13	1:A:363:ILE:HD11	1.79	0.64
7:G:71:VAL:HG13	7:G:72:LYS:H	1.62	0.64
5:E:145:CYS:C	5:E:147:LYS:H	2.05	0.64
1:A:92:PHE:O	1:A:96:VAL:HG23	1.98	0.64
5:E:139:GLU:OE1	5:E:142:LEU:HD21	1.98	0.64
2:B:283:PHE:O	2:B:287:GLN:HG2	1.98	0.63
1:A:104:GLU:OE1	1:A:105:PRO:HD2	1.98	0.63
3:C:27:PRO:HG2	3:C:29:ASN:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HG3	1:A:72:TYR:CE2	2.33	0.63
2:B:320:GLU:O	2:B:323:GLN:HB2	1.99	0.63
5:E:59:GLU:OE1	5:E:61:LYS:HE2	1.99	0.63
3:C:12:SER:HB2	3:C:26:CYS:HB3	1.80	0.63
2:B:318:GLU:HG3	2:B:344:ILE:HD12	1.80	0.62
5:E:85:CYS:HB2	5:E:90:GLN:NE2	2.14	0.62
2:B:254:VAL:HG12	2:B:258:ARG:HG3	1.81	0.62
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.82	0.62
1:A:87:ASP:OD2	4:D:267:ARG:HD2	1.99	0.62
2:B:175:LEU:CD1	2:B:178:LEU:HD12	2.30	0.62
4:D:203:ARG:O	4:D:216:VAL:HG13	1.98	0.62
1:A:352:GLU:C	1:A:353:LEU:HD22	2.24	0.62
3:C:107:ASN:ND2	3:C:107:ASN:C	2.58	0.62
4:D:158:LYS:HD3	4:D:158:LYS:C	2.25	0.62
5:E:139:GLU:O	5:E:142:LEU:HD23	1.99	0.62
5:E:144:LEU:O	5:E:148:VAL:HG23	1.99	0.62
7:G:58:ALA:HB1	7:G:79:VAL:HG22	1.82	0.62
3:C:183:THR:HB	3:C:189:MET:CE	2.29	0.62
5:E:16:ILE:HG23	5:E:16:ILE:O	1.99	0.61
1:A:343:VAL:HG23	1:A:346:ARG:NH2	2.14	0.61
3:C:272:TYR:CE1	3:C:277:GLY:HA2	2.34	0.61
2:B:217:LYS:HG3	2:B:221:CYS:SG	2.41	0.61
2:B:259:PHE:O	2:B:262:PRO:HD2	2.01	0.61
4:D:263:HIS:HB3	4:D:267:ARG:HH12	1.65	0.61
7:G:104:ASP:OD2	7:G:143:ARG:NE	2.24	0.61
1:A:186:ILE:O	1:A:186:ILE:HG22	1.99	0.61
3:C:79:TRP:CZ3	3:C:88:PRO:HB3	2.36	0.61
4:D:140:ASN:H	4:D:140:ASN:ND2	1.99	0.61
4:D:233:ASN:OD1	4:D:235:SER:HB3	2.01	0.61
4:D:269:LYS:HE2	6:F:145:GLU:HB2	1.83	0.61
7:G:124:VAL:O	7:G:127:GLN:HB2	2.01	0.61
4:D:198:VAL:C	4:D:199:LEU:HD12	2.25	0.60
1:A:36:ALA:HA	1:A:73:ALA:O	2.01	0.60
2:B:239:VAL:HG23	2:B:240:LEU:CD1	2.31	0.60
7:G:8:SER:C	7:G:10:ARG:H	2.07	0.60
7:G:79:VAL:HG21	7:G:109:TYR:CD1	2.36	0.60
1:A:194:PRO:C	1:A:195:ILE:HD12	2.27	0.60
2:B:202:TYR:CE1	2:B:252:ILE:HB	2.36	0.60
3:C:21:THR:HG23	3:C:22:GLN:HG3	1.83	0.60
4:D:60:SER:HB2	4:D:91:TYR:CD2	2.37	0.60
5:E:50:LYS:NZ	5:E:159:TRP:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:LEU:HD13	5:E:98:LEU:O	2.02	0.60
3:C:90:LEU:HD23	3:C:91:VAL:N	2.17	0.60
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.01	0.60
7:G:71:VAL:HG13	7:G:72:LYS:N	2.17	0.59
4:D:169:PHE:O	4:D:219:ASN:HB3	2.02	0.59
1:A:87:ASP:CG	4:D:264:THR:HG22	2.27	0.59
1:A:19:LEU:CD1	1:A:96:VAL:HG13	2.31	0.59
1:A:25:THR:O	1:A:25:THR:HG22	2.01	0.59
6:F:51:VAL:HB	7:G:111:TYR:HD2	1.67	0.59
5:E:22:LEU:HD23	5:E:41:ILE:HB	1.84	0.59
7:G:105:LEU:O	7:G:108:LYS:HB2	2.02	0.59
3:C:26:CYS:SG	3:C:55:VAL:HB	2.43	0.59
4:D:277:LEU:HD23	6:F:134:PHE:CZ	2.37	0.59
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.17	0.59
7:G:103:VAL:HG11	7:G:136:GLY:CA	2.33	0.59
4:D:261:TYR:HE2	6:F:152:SER:HG	1.50	0.59
1:A:12:CYS:HB3	1:A:78:ILE:HD13	1.85	0.59
4:D:147:ARG:HD3	4:D:150:GLU:CD	2.27	0.59
5:E:157:SER:C	5:E:159:TRP:H	2.11	0.59
5:E:169:MET:O	5:E:171:LYS:HG2	2.03	0.59
6:F:15:THR:OG1	7:G:111:TYR:OH	2.21	0.59
6:F:76:VAL:HG12	6:F:77:LYS:N	2.17	0.59
3:C:144:THR:CB	6:F:28:GLN:HE21	2.15	0.58
4:D:223:ILE:HD12	4:D:223:ILE:N	2.18	0.58
2:B:163:VAL:CA	2:B:185:ALA:HB2	2.30	0.58
6:F:76:VAL:HG12	6:F:77:LYS:H	1.68	0.58
1:A:64:ASP:C	1:A:66:ALA:H	2.11	0.58
1:A:349:LEU:O	1:A:353:LEU:HD23	2.02	0.58
5:E:18:ASN:ND2	5:E:66:ARG:HD2	2.19	0.58
1:A:28:GLN:CG	4:D:10:ILE:HD13	2.33	0.58
1:A:17:THR:HG22	1:A:19:LEU:HD22	1.85	0.58
1:A:262:ILE:HG22	1:A:263:SER:N	2.17	0.58
1:A:230:ARG:HH11	1:A:230:ARG:CB	2.17	0.58
7:G:103:VAL:HG11	7:G:136:GLY:HA3	1.86	0.58
2:B:165:HIS:HD2	2:B:181:ARG:HG2	1.68	0.58
4:D:223:ILE:HG21	4:D:247:PHE:CZ	2.39	0.58
5:E:87:SER:HA	5:E:153:ASN:OD1	2.04	0.58
1:A:321:LEU:HD12	1:A:369:THR:HG22	1.86	0.57
3:C:13:CYS:HA	3:C:331:GLN:NE2	2.18	0.57
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.85	0.57
3:C:3:TYR:CD1	3:C:4:HIS:N	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:LYS:O	5:E:92:GLU:HG3	2.05	0.57
7:G:109:TYR:HE2	7:G:151:VAL:HG11	1.69	0.57
1:A:363:ILE:HD13	1:A:363:ILE:N	2.14	0.57
4:D:135:GLY:O	4:D:137:GLU:HG3	2.04	0.57
8:A:501:C69:OAA	8:A:501:C69:CAG	2.52	0.57
3:C:19:ASP:O	3:C:20:ARG:HB2	2.03	0.57
3:C:118:ARG:HH11	3:C:118:ARG:HG3	1.68	0.57
4:D:91:TYR:CD1	4:D:91:TYR:N	2.72	0.57
4:D:233:ASN:OD1	4:D:235:SER:N	2.37	0.57
5:E:66:ARG:HG3	5:E:66:ARG:HH11	1.68	0.57
2:B:322:LYS:CG	2:B:342:ILE:HD11	2.34	0.57
3:C:96:ASN:OD1	3:C:97:ARG:HG2	2.04	0.57
6:F:60:LYS:HE3	6:F:112:TYR:CE2	2.39	0.57
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.40	0.57
3:C:105:ALA:HA	3:C:150:TRP:CD1	2.40	0.57
4:D:65:LYS:HE2	4:D:65:LYS:H	1.68	0.57
1:A:37:ILE:C	1:A:37:ILE:HD12	2.30	0.57
1:A:38:LYS:HD2	1:A:59:ASP:OD1	2.04	0.57
3:C:272:TYR:HE1	3:C:277:GLY:HA2	1.68	0.57
4:D:223:ILE:HD12	4:D:223:ILE:H	1.70	0.56
6:F:93:PHE:CE1	6:F:97:ARG:NH1	2.73	0.56
1:A:98:PHE:CD1	4:D:253:TYR:CD1	2.93	0.56
2:B:322:LYS:HG3	2:B:342:ILE:HD11	1.87	0.56
3:C:357:TRP:N	3:C:357:TRP:CD1	2.73	0.56
5:E:56:LYS:O	5:E:169:MET:HA	2.06	0.56
5:E:31:PRO:CG	5:E:132:TYR:HB2	2.32	0.56
1:A:389:GLU:OE1	1:A:414:PHE:HB2	2.05	0.56
5:E:5:HIS:HA	5:E:58:TYR:OH	2.06	0.56
5:E:82:LEU:HD13	5:E:95:MET:SD	2.46	0.56
6:F:146:ILE:HA	6:F:149:MET:CE	2.34	0.56
1:A:99:LYS:HD3	1:A:100:TYR:HE2	1.69	0.56
2:B:263:GLU:HG3	2:B:263:GLU:O	2.05	0.56
4:D:181:PHE:CE2	6:F:157:ALA:HA	2.41	0.56
1:A:190:ILE:O	1:A:191:LYS:HD2	2.06	0.55
1:A:211:ARG:NH1	5:E:159:TRP:CZ3	2.74	0.55
3:C:327:ASN:H	3:C:351:ASP:HB3	1.71	0.55
4:D:267:ARG:HG3	4:D:267:ARG:HH11	1.72	0.55
7:G:74:ARG:O	7:G:78:ILE:HG13	2.06	0.55
2:B:235:LEU:O	6:F:106:ARG:HD2	2.06	0.55
3:C:114:GLY:H	3:C:148:LEU:HD11	1.71	0.55
3:C:131:TRP:HE3	3:C:131:TRP:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:ARG:HD3	4:D:150:GLU:OE2	2.06	0.55
1:A:185:VAL:O	1:A:187:GLY:N	2.37	0.55
5:E:74:TYR:O	5:E:77:GLU:HB2	2.06	0.55
7:G:54:ALA:O	7:G:57:ALA:HB3	2.06	0.55
2:B:236:GLU:HB3	6:F:105:ARG:NH1	2.19	0.55
3:C:27:PRO:HG2	3:C:29:ASN:HB3	1.87	0.55
3:C:266:PHE:HB2	3:C:286:ASP:HB3	1.89	0.55
1:A:112:LEU:CD1	1:A:130:MET:HE2	2.26	0.55
3:C:27:PRO:C	3:C:29:ASN:H	2.15	0.55
4:D:59:ILE:HD13	4:D:61:LEU:HD11	1.88	0.55
4:D:265:ARG:NH1	4:D:265:ARG:HG2	2.22	0.55
6:F:107:LYS:HG3	6:F:108:PRO:HD2	1.89	0.55
3:C:15:ALA:HB3	3:C:58:ILE:HG22	1.88	0.55
4:D:43:TYR:OH	4:D:117:LYS:HB2	2.07	0.55
5:E:28:PHE:CE2	5:E:138:GLN:HB3	2.42	0.55
3:C:97:ARG:NE	6:F:28:GLN:O	2.30	0.55
4:D:223:ILE:HG21	4:D:247:PHE:CE2	2.41	0.55
4:D:265:ARG:HG2	4:D:265:ARG:HH11	1.71	0.55
6:F:53:ILE:HA	7:G:114:PHE:CD1	2.41	0.55
2:B:298:TYR:CD1	2:B:340:PHE:HE1	2.24	0.55
1:A:69:LYS:HB3	1:A:72:TYR:HB2	1.88	0.54
1:A:274:GLU:N	1:A:274:GLU:OE1	2.40	0.54
2:B:223:VAL:HG21	2:B:313:LEU:HD13	1.89	0.54
3:C:16:TRP:CE2	3:C:335:LEU:HD21	2.42	0.54
6:F:95:MET:CE	6:F:108:PRO:HG3	2.37	0.54
1:A:80:HIS:HE1	1:A:192:HIS:CE1	2.25	0.54
1:A:343:VAL:HG22	1:A:363:ILE:HG13	1.89	0.54
3:C:359:VAL:O	3:C:363:GLU:HG3	2.07	0.54
4:D:247:PHE:O	4:D:250:TYR:N	2.40	0.54
6:F:109:VAL:O	6:F:110:GLU:C	2.50	0.54
1:A:211:ARG:NH1	5:E:159:TRP:HZ3	2.05	0.54
2:B:158:ASP:HA	2:B:304:SER:O	2.07	0.54
3:C:335:LEU:HB2	3:C:344:GLN:O	2.07	0.54
4:D:9:ARG:HG2	4:D:9:ARG:NH1	2.23	0.54
2:B:239:VAL:HG23	2:B:240:LEU:HD12	1.89	0.54
3:C:79:TRP:CE3	3:C:88:PRO:HB3	2.43	0.54
6:F:39:GLU:O	6:F:41:ARG:HG3	2.08	0.54
7:G:68:SER:CB	7:G:71:VAL:HG12	2.37	0.54
3:C:70:CYS:HB2	3:C:99:ALA:HB1	1.90	0.54
4:D:68:GLN:HA	4:D:72:ALA:HB3	1.90	0.54
5:E:13:THR:HG21	5:E:22:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:79:VAL:HG11	7:G:109:TYR:CD1	2.43	0.54
2:B:223:VAL:HG12	2:B:224:GLY:O	2.08	0.54
3:C:227:CYS:SG	3:C:239:THR:HG23	2.48	0.54
3:C:119:VAL:HG23	3:C:138:LYS:HA	1.90	0.53
6:F:141:GLU:OE1	6:F:144:LYS:HD2	2.08	0.53
4:D:248:ARG:HD3	4:D:248:ARG:C	2.32	0.53
3:C:226:VAL:HG12	3:C:240:LEU:HB3	1.89	0.53
3:C:254:THR:OG1	3:C:372:VAL:HG22	2.09	0.53
4:D:129:PHE:CE1	4:D:232:THR:HG22	2.44	0.53
5:E:70:TYR:CE2	5:E:133:LEU:HG	2.43	0.53
6:F:95:MET:HE1	6:F:108:PRO:CG	2.36	0.53
1:A:87:ASP:OD2	4:D:264:THR:HG22	2.08	0.53
1:A:308:PRO:HG3	2:B:208:ALA:HB2	1.90	0.53
3:C:14:HIS:N	3:C:331:GLN:HE22	2.03	0.53
3:C:122:ILE:O	3:C:134:CYS:HB2	2.09	0.53
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.74	0.53
7:G:109:TYR:CE2	7:G:151:VAL:HG21	2.44	0.53
1:A:21:TYR:OH	1:A:103:ALA:HB2	2.08	0.53
1:A:69:LYS:HB3	1:A:72:TYR:CD1	2.43	0.53
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.89	0.53
5:E:152:GLN:O	5:E:155:LYS:HD2	2.08	0.53
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.43	0.53
2:B:281:LEU:O	2:B:281:LEU:HD23	2.08	0.53
5:E:10:ASP:C	5:E:12:ASP:H	2.15	0.53
3:C:209:CYS:SG	3:C:251:THR:HA	2.49	0.53
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.44	0.53
7:G:75:ALA:O	7:G:79:VAL:HG23	2.08	0.53
1:A:52:MET:HE1	9:A:611:HOH:O	2.09	0.52
1:A:218:GLU:C	1:A:220:SER:H	2.16	0.52
2:B:278:VAL:CG1	2:B:279:ALA:N	2.72	0.52
3:C:204:TRP:O	3:C:221:SER:HA	2.09	0.52
4:D:158:LYS:HD3	4:D:158:LYS:O	2.10	0.52
1:A:337:ARG:HD2	1:A:341:ARG:NH2	2.24	0.52
2:B:329:VAL:HG12	2:B:329:VAL:O	2.08	0.52
7:G:91:ILE:O	7:G:95:VAL:HG23	2.09	0.52
1:A:84:GLU:HB3	8:A:501:C69:CAL	2.39	0.52
2:B:163:VAL:HG22	2:B:164:THR:N	2.24	0.52
2:B:266:PHE:HD1	2:B:320:GLU:OE2	1.92	0.52
4:D:75:LEU:HD23	4:D:75:LEU:C	2.35	0.52
3:C:226:VAL:CG1	3:C:240:LEU:HB3	2.39	0.52
7:G:36:GLY:HA2	7:G:63:PRO:HG3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG23	6:F:159:ILE:HD12	1.91	0.52
3:C:27:PRO:C	3:C:29:ASN:N	2.66	0.52
7:G:11:PHE:CE1	7:G:12:ARG:HG2	2.45	0.52
3:C:114:GLY:N	3:C:148:LEU:HD11	2.25	0.52
4:D:65:LYS:HZ2	4:D:65:LYS:CB	2.22	0.52
4:D:80:TYR:OH	4:D:119:ASN:ND2	2.37	0.52
1:A:334:ARG:HH11	1:A:334:ARG:HG2	1.74	0.52
4:D:143:VAL:HG12	4:D:143:VAL:O	2.08	0.52
1:A:57:ASP:CG	6:F:156:ARG:HH12	2.18	0.52
2:B:175:LEU:HD23	2:B:175:LEU:H	1.73	0.52
2:B:286:ILE:HG21	2:B:298:TYR:CE2	2.44	0.52
5:E:126:ASP:O	5:E:130:ARG:HB2	2.09	0.52
1:A:309:ILE:HG23	1:A:310:ASP:N	2.25	0.52
3:C:107:ASN:ND2	3:C:109:LYS:N	2.47	0.52
1:A:393:VAL:HG23	1:A:393:VAL:O	2.10	0.51
3:C:116:GLY:C	3:C:118:ARG:N	2.67	0.51
4:D:277:LEU:HD23	6:F:134:PHE:CE2	2.45	0.51
1:A:183:GLY:HA3	1:A:413:VAL:HG21	1.92	0.51
3:C:218:ALA:HA	3:C:227:CYS:O	2.09	0.51
5:E:30:GLY:HA3	5:E:135:GLN:CD	2.35	0.51
6:F:8:TYR:OH	6:F:61:VAL:HG23	2.11	0.51
6:F:52:THR:O	7:G:114:PHE:HB3	2.10	0.51
2:B:278:VAL:HG13	2:B:279:ALA:H	1.76	0.51
3:C:354:MET:C	3:C:354:MET:SD	2.94	0.51
4:D:202:HIS:O	4:D:204:GLU:N	2.36	0.51
1:A:327:MET:O	1:A:328:PHE:C	2.53	0.51
2:B:189:ILE:HG23	2:B:261:ALA:O	2.11	0.51
3:C:172:TYR:C	3:C:172:TYR:CD2	2.88	0.51
1:A:347:LEU:HD22	1:A:363:ILE:HD12	1.92	0.51
4:D:180:VAL:HG11	6:F:153:VAL:HG12	1.92	0.51
4:D:181:PHE:CD2	6:F:157:ALA:HA	2.44	0.51
1:A:37:ILE:HB	9:A:611:HOH:O	2.10	0.51
1:A:225:LYS:O	1:A:229:GLU:HG3	2.10	0.51
1:A:351:GLU:C	1:A:353:LEU:H	2.18	0.51
2:B:217:LYS:O	2:B:221:CYS:HB2	2.11	0.51
1:A:254:LYS:HE2	1:A:275:ARG:NH1	2.25	0.51
3:C:211:SER:HB3	3:C:216:ARG:HB2	1.92	0.51
3:C:265:CYS:SG	3:C:327:ASN:C	2.94	0.51
5:E:6:SER:HB2	5:E:68:LEU:HD22	1.91	0.51
5:E:97:THR:O	5:E:101:THR:HG23	2.10	0.51
8:A:501:C69:OAW	8:A:501:C69:CAP	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:ASN:OD1	3:C:31:GLU:N	2.43	0.51
3:C:131:TRP:O	3:C:131:TRP:CE3	2.63	0.51
2:B:277:GLY:O	2:B:279:ALA:N	2.44	0.51
4:D:5:GLU:OE1	4:D:9:ARG:NE	2.36	0.51
4:D:132:GLN:HB2	4:D:156:SER:OG	2.11	0.51
4:D:160:ARG:HB3	4:D:160:ARG:NH1	2.25	0.51
1:A:100:TYR:N	1:A:100:TYR:CD2	2.79	0.51
4:D:266:MET:HE3	6:F:93:PHE:CG	2.46	0.51
1:A:112:LEU:HD11	1:A:130:MET:CE	2.27	0.50
5:E:85:CYS:SG	5:E:149:PHE:HZ	2.34	0.50
5:E:132:TYR:O	5:E:132:TYR:CG	2.63	0.50
6:F:85:ILE:HD12	6:F:85:ILE:C	2.35	0.50
1:A:145:ALA:O	1:A:167:VAL:HG21	2.11	0.50
4:D:37:ASP:HB2	4:D:43:TYR:HE1	1.77	0.50
6:F:130:LYS:O	6:F:133:ASP:HB2	2.12	0.50
6:F:107:LYS:HG3	6:F:108:PRO:CD	2.42	0.50
1:A:334:ARG:HD2	1:A:337:ARG:HH21	1.77	0.50
2:B:183:ASP:C	2:B:184:ILE:HG13	2.35	0.50
5:E:99:GLY:O	5:E:134:GLN:HG3	2.11	0.50
6:F:141:GLU:OE1	6:F:141:GLU:HA	2.10	0.50
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.75	0.50
2:B:231:GLN:HA	2:B:231:GLN:NE2	2.27	0.50
1:A:102:ARG:C	4:D:38:PHE:CE2	2.89	0.50
3:C:15:ALA:CB	3:C:58:ILE:HG22	2.41	0.50
3:C:196:PHE:HB2	3:C:235:MET:HE2	1.93	0.50
7:G:66:THR:O	7:G:72:LYS:HE3	2.12	0.50
1:A:111:LEU:C	1:A:111:LEU:CD2	2.84	0.49
3:C:7:LEU:O	3:C:352:GLY:HA3	2.12	0.49
3:C:343:SER:C	3:C:359:VAL:HG23	2.37	0.49
1:A:327:MET:CE	1:A:374:ARG:HB2	2.30	0.49
1:A:146:VAL:O	1:A:149:LEU:HB2	2.13	0.49
3:C:6:PHE:HE2	3:C:35:TYR:CG	2.29	0.49
5:E:25:ARG:O	5:E:139:GLU:OE2	2.29	0.49
4:D:141:ARG:HB3	4:D:155:GLU:HB3	1.93	0.49
5:E:5:HIS:HD2	5:E:65:ASP:OD2	1.96	0.49
2:B:198:LEU:C	2:B:200:ARG:H	2.20	0.49
3:C:166:CYS:H	3:C:198:SER:HG	1.61	0.49
3:C:240:LEU:HD23	3:C:270:PHE:HE2	1.78	0.49
3:C:256:SER:HB2	3:C:372:VAL:HG13	1.94	0.49
4:D:269:LYS:HG2	6:F:145:GLU:HG2	1.95	0.49
4:D:45:ILE:HA	4:D:56:MET:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:OE1	1:A:105:PRO:CD	2.61	0.49
5:E:5:HIS:HA	5:E:58:TYR:HH	1.78	0.49
1:A:101:LEU:O	1:A:102:ARG:C	2.56	0.49
6:F:38:VAL:HG12	6:F:69:SER:OG	2.12	0.49
2:B:231:GLN:HA	2:B:231:GLN:HE21	1.77	0.48
4:D:5:GLU:CD	4:D:9:ARG:HE	2.19	0.48
4:D:130:GLN:OE1	4:D:130:GLN:HA	2.13	0.48
4:D:263:HIS:HB3	4:D:267:ARG:NH1	2.27	0.48
1:A:305:GLN:OE1	1:A:305:GLN:HA	2.13	0.48
1:A:384:LEU:O	1:A:390:PHE:HB2	2.13	0.48
1:A:116:PRO:O	1:A:117:LEU:HB2	2.13	0.48
3:C:125:PHE:HD2	3:C:132:TRP:NE1	2.11	0.48
5:E:8:LEU:HD12	5:E:41:ILE:HB	1.94	0.48
6:F:158:ARG:O	6:F:162:GLU:HG3	2.13	0.48
3:C:30:HIS:HB2	9:C:423:HOH:O	2.14	0.48
5:E:18:ASN:HD21	5:E:117:TYR:HA	1.79	0.48
3:C:27:PRO:HG2	3:C:29:ASN:HB2	1.95	0.48
4:D:53:THR:C	4:D:54:LYS:HD2	2.38	0.48
4:D:147:ARG:O	4:D:148:ASP:C	2.55	0.48
5:E:152:GLN:CB	5:E:155:LYS:NZ	2.77	0.48
6:F:68:ASN:O	6:F:69:SER:HB3	2.14	0.48
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.43	0.48
2:B:326:LEU:HD23	2:B:327:GLU:N	2.27	0.48
3:C:219:TRP:CE2	3:C:227:CYS:HB2	2.48	0.48
4:D:2:ILE:O	4:D:250:TYR:HE1	1.97	0.48
6:F:77:LYS:C	6:F:78:GLN:HG3	2.38	0.48
1:A:334:ARG:CD	1:A:337:ARG:HH21	2.26	0.48
3:C:273:ASP:OD1	3:C:275:ALA:HB3	2.13	0.48
4:D:228:PHE:O	4:D:229:PRO:C	2.57	0.48
1:A:25:THR:O	1:A:25:THR:CG2	2.62	0.48
1:A:231:TYR:CD1	1:A:254:LYS:HG3	2.49	0.48
2:B:178:LEU:HD21	2:B:288:ALA:O	2.13	0.48
3:C:284:ARG:NH1	3:C:286:ASP:O	2.42	0.48
5:E:93:LYS:O	5:E:96:TYR:HB3	2.13	0.48
6:F:60:LYS:HE3	6:F:112:TYR:OH	2.14	0.48
2:B:166:ILE:O	2:B:168:PRO:HD3	2.13	0.48
4:D:32:GLU:OE2	4:D:44:HIS:NE2	2.37	0.48
3:C:254:THR:HG21	3:C:372:VAL:CG2	2.44	0.47
4:D:35:PHE:CE1	4:D:43:TYR:CD1	3.02	0.47
4:D:243:LEU:HD12	6:F:168:PHE:CD1	2.49	0.47
2:B:308:THR:O	2:B:313:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:ASN:ND2	3:C:131:TRP:CH2	2.82	0.47
5:E:58:TYR:HB3	5:E:169:MET:SD	2.55	0.47
5:E:80:LYS:HA	5:E:164:VAL:CG2	2.44	0.47
5:E:85:CYS:HB2	5:E:90:GLN:CD	2.38	0.47
1:A:15:GLY:O	1:A:32:PRO:HA	2.15	0.47
1:A:215:ILE:HD11	1:A:269:ILE:HG21	1.96	0.47
3:C:100:ARG:NH2	6:F:23:GLU:OE2	2.47	0.47
4:D:61:LEU:HD23	4:D:63:PHE:CZ	2.49	0.47
1:A:189:CYS:SG	1:A:306:ASN:O	2.60	0.47
1:A:324:GLY:O	1:A:327:MET:HG2	2.14	0.47
5:E:112:PRO:O	5:E:113:LEU:HB2	2.14	0.47
6:F:145:GLU:O	6:F:149:MET:HG3	2.14	0.47
1:A:69:LYS:HD2	1:A:72:TYR:CD1	2.50	0.47
1:A:157:GLN:HE22	1:A:369:THR:H	1.63	0.47
7:G:109:TYR:CE2	7:G:151:VAL:HG11	2.49	0.47
2:B:161:ASP:HA	2:B:186:GLY:HA3	1.95	0.47
3:C:126:GLU:C	3:C:128:GLU:H	2.22	0.47
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.96	0.47
4:D:247:PHE:O	4:D:248:ARG:C	2.58	0.47
4:D:277:LEU:CD1	6:F:102:PHE:HE1	2.28	0.47
5:E:66:ARG:HB3	5:E:117:TYR:CE2	2.50	0.47
7:G:8:SER:C	7:G:10:ARG:N	2.72	0.47
1:A:164:THR:HA	1:A:180:VAL:O	2.14	0.47
1:A:230:ARG:NH1	1:A:231:TYR:CE2	2.83	0.47
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.45	0.47
3:C:144:THR:OG1	6:F:28:GLN:HG2	2.15	0.47
4:D:267:ARG:HG3	4:D:267:ARG:NH1	2.30	0.47
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.77	0.47
2:B:337:LEU:CD1	7:G:16:VAL:HG13	2.44	0.47
3:C:167:ARG:CG	3:C:197:GLU:HG3	2.44	0.47
4:D:178:GLY:HA2	4:D:255:ILE:HD11	1.96	0.47
4:D:189:ARG:NH2	4:D:197:GLN:HG3	2.30	0.47
5:E:91:GLY:C	5:E:93:LYS:N	2.73	0.47
5:E:150:ASP:C	5:E:152:GLN:N	2.71	0.47
1:A:395:HIS:CE1	1:A:410:HIS:O	2.68	0.47
2:B:205:ASN:HB3	2:B:208:ALA:HB3	1.97	0.47
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.97	0.47
1:A:239:VAL:HG23	1:A:240:LYS:N	2.30	0.46
2:B:230:GLU:OE2	6:F:35:LYS:HE2	2.14	0.46
4:D:175:VAL:HG11	4:D:202:HIS:HE1	1.81	0.46
6:F:93:PHE:CE1	6:F:97:ARG:CZ	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HB3	8:A:501:C69:OAW	2.16	0.46
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.96	0.46
4:D:113:ALA:O	4:D:116:LEU:HB2	2.15	0.46
4:D:152:MET:HE3	4:D:154:VAL:HG23	1.97	0.46
7:G:75:ALA:HA	7:G:78:ILE:HD12	1.96	0.46
4:D:229:PRO:C	4:D:231:HIS:H	2.23	0.46
4:D:229:PRO:O	4:D:231:HIS:N	2.48	0.46
6:F:81:GLU:O	6:F:85:ILE:HG23	2.14	0.46
7:G:11:PHE:O	7:G:14:VAL:HG12	2.15	0.46
1:A:69:LYS:HB3	1:A:72:TYR:HD1	1.79	0.46
2:B:252:ILE:HG13	2:B:253:LYS:N	2.29	0.46
3:C:118:ARG:HA	3:C:143:SER:O	2.14	0.46
5:E:131:ALA:C	5:E:133:LEU:H	2.23	0.46
2:B:282:LEU:CD2	2:B:321:LEU:HD11	2.44	0.46
4:D:67:LEU:HD22	4:D:120:CYS:O	2.15	0.46
1:A:86:TRP:CB	4:D:267:ARG:HE	2.29	0.46
1:A:228:LYS:O	1:A:232:SER:HB2	2.15	0.46
3:C:21:THR:CG2	3:C:22:GLN:HG3	2.44	0.46
4:D:10:ILE:O	4:D:14:THR:OG1	2.21	0.46
4:D:247:PHE:O	4:D:250:TYR:HB3	2.16	0.46
1:A:86:TRP:HB2	4:D:267:ARG:HE	1.81	0.46
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.51	0.46
4:D:116:LEU:C	4:D:116:LEU:HD23	2.41	0.46
5:E:5:HIS:CD2	5:E:65:ASP:OD2	2.69	0.46
2:B:326:LEU:HD23	2:B:326:LEU:C	2.41	0.46
3:C:100:ARG:O	3:C:100:ARG:HG3	2.16	0.46
4:D:65:LYS:H	4:D:65:LYS:CE	2.29	0.46
1:A:153:TRP:HE1	1:A:162:THR:H	1.63	0.46
1:A:177:VAL:CG1	1:A:300:VAL:HG22	2.46	0.46
1:A:230:ARG:HH11	1:A:230:ARG:HB3	1.79	0.46
1:A:309:ILE:HG23	1:A:310:ASP:H	1.80	0.46
3:C:59:ASP:OD1	3:C:103:ARG:HD3	2.15	0.46
3:C:105:ALA:HB2	3:C:150:TRP:CE2	2.51	0.46
5:E:145:CYS:C	5:E:147:LYS:N	2.72	0.46
1:A:144:GLN:O	1:A:145:ALA:C	2.59	0.45
1:A:194:PRO:O	1:A:195:ILE:HD12	2.16	0.45
1:A:347:LEU:HD21	1:A:363:ILE:HG23	1.97	0.45
2:B:259:PHE:CE2	2:B:260:GLU:HG3	2.51	0.45
3:C:73:ASP:OD1	3:C:73:ASP:N	2.49	0.45
1:A:6:PRO:HG2	1:A:21:TYR:HD2	1.81	0.45
1:A:334:ARG:HG2	1:A:334:ARG:NH1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:188:GLY:C	4:D:190:ARG:H	2.25	0.45
5:E:152:GLN:O	5:E:153:ASN:O	2.35	0.45
1:A:154:THR:HG23	1:A:155:SER:N	2.31	0.45
1:A:395:HIS:HE1	1:A:410:HIS:O	1.98	0.45
2:B:217:LYS:HA	2:B:221:CYS:SG	2.57	0.45
3:C:263:HIS:HA	3:C:328:SER:OG	2.16	0.45
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.51	0.45
4:D:205:PRO:HD2	4:D:216:VAL:HG22	1.97	0.45
5:E:60:ILE:N	5:E:60:ILE:HD12	2.30	0.45
2:B:255:GLY:O	2:B:256:GLY:C	2.60	0.45
4:D:281:ARG:HH12	6:F:126:MET:HE2	1.76	0.45
5:E:13:THR:HG21	5:E:22:LEU:CD1	2.47	0.45
5:E:28:PHE:CD2	5:E:138:GLN:HB3	2.51	0.45
7:G:68:SER:OG	7:G:71:VAL:HG12	2.16	0.45
4:D:154:VAL:HG12	4:D:155:GLU:N	2.31	0.45
6:F:74:ILE:HD13	6:F:139:MET:HG2	1.99	0.45
1:A:113:THR:HB	1:A:144:GLN:HG3	1.99	0.45
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.46	0.45
4:D:59:ILE:CD1	4:D:61:LEU:HD11	2.46	0.45
1:A:106:GLU:HG3	1:A:135:ASN:HB2	1.99	0.45
1:A:193:ILE:HA	1:A:194:PRO:HD3	1.79	0.45
2:B:189:ILE:HD11	2:B:265:LEU:HG	1.97	0.45
3:C:269:LEU:O	3:C:282:GLY:N	2.43	0.45
5:E:134:GLN:O	5:E:138:GLN:HG2	2.17	0.45
6:F:51:VAL:HB	7:G:111:TYR:CD2	2.48	0.45
1:A:157:GLN:NE2	1:A:369:THR:H	2.14	0.45
3:C:151:HIS:HA	3:C:210:PHE:CD1	2.51	0.45
3:C:240:LEU:HD23	3:C:270:PHE:CD2	2.51	0.45
1:A:60:PHE:CZ	1:A:91:ARG:HB3	2.52	0.45
3:C:27:PRO:HG3	3:C:33:HIS:HD2	1.75	0.45
3:C:32:VAL:CG2	3:C:58:ILE:HD11	2.41	0.45
3:C:329:VAL:HG11	3:C:347:THR:HB	1.98	0.45
4:D:51:ASP:OD1	4:D:54:LYS:HD3	2.16	0.45
5:E:172:SER:C	5:E:174:SER:H	2.25	0.45
6:F:8:TYR:CE2	6:F:139:MET:HE1	2.53	0.45
1:A:272:GLY:C	1:A:274:GLU:OE1	2.60	0.44
2:B:198:LEU:C	2:B:200:ARG:N	2.75	0.44
3:C:6:PHE:O	3:C:7:LEU:HB3	2.17	0.44
4:D:205:PRO:HA	4:D:206:PRO:HD3	1.83	0.44
4:D:236:ALA:O	4:D:238:ASP:N	2.50	0.44
5:E:139:GLU:OE1	5:E:139:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PRO:HG2	1:A:21:TYR:CD2	2.53	0.44
1:A:68:GLU:O	1:A:69:LYS:C	2.59	0.44
1:A:258:GLY:C	1:A:259:ILE:HD12	2.40	0.44
4:D:116:LEU:C	4:D:116:LEU:CD2	2.91	0.44
4:D:189:ARG:NH1	4:D:197:GLN:HG3	2.30	0.44
5:E:139:GLU:HA	5:E:142:LEU:CD2	2.47	0.44
5:E:157:SER:C	5:E:159:TRP:N	2.73	0.44
1:A:144:GLN:O	1:A:146:VAL:N	2.51	0.44
2:B:236:GLU:O	6:F:105:ARG:HG2	2.17	0.44
3:C:254:THR:HG1	3:C:372:VAL:HG22	1.81	0.44
5:E:85:CYS:CB	5:E:90:GLN:HE22	2.30	0.44
7:G:39:GLU:O	7:G:40:GLY:C	2.60	0.44
3:C:265:CYS:SG	3:C:327:ASN:O	2.76	0.44
3:C:266:PHE:CD1	3:C:266:PHE:C	2.95	0.44
1:A:284:HIS:N	1:A:285:PRO:HD3	2.33	0.44
1:A:390:PHE:O	1:A:394:CYS:HB2	2.18	0.44
2:B:175:LEU:N	2:B:175:LEU:CD2	2.81	0.44
2:B:231:GLN:HE21	2:B:231:GLN:CA	2.30	0.44
2:B:278:VAL:CG1	2:B:279:ALA:H	2.30	0.44
4:D:241:ILE:HA	4:D:244:ILE:HG22	2.00	0.44
6:F:102:PHE:CD1	6:F:102:PHE:N	2.84	0.44
1:A:154:THR:CG2	1:A:155:SER:N	2.81	0.44
1:A:216:PRO:HG2	1:A:219:GLN:OE1	2.18	0.44
3:C:30:HIS:C	3:C:31:GLU:HG3	2.42	0.44
3:C:160:GLY:HA3	3:C:205:VAL:CG1	2.48	0.44
4:D:146:TYR:CD1	4:D:147:ARG:HG3	2.53	0.44
4:D:202:HIS:C	4:D:204:GLU:H	2.24	0.44
5:E:49:PHE:O	5:E:53:VAL:HG12	2.18	0.44
6:F:120:ASN:O	6:F:124:GLU:HB2	2.18	0.44
2:B:227:ILE:HG13	2:B:263:GLU:OE1	2.18	0.44
3:C:185:TRP:HE3	3:C:235:MET:HE3	1.83	0.44
4:D:87:PRO:HB3	4:D:92:ASN:O	2.18	0.44
4:D:109:ILE:HG13	4:D:110:VAL:N	2.32	0.44
7:G:100:LYS:HD3	7:G:100:LYS:HA	1.72	0.44
2:B:190:THR:O	2:B:193:LEU:HB3	2.17	0.44
2:B:232:LYS:NZ	2:B:232:LYS:HB3	2.33	0.44
2:B:322:LYS:HD2	7:G:16:VAL:HG11	1.99	0.44
3:C:201:SER:HB3	7:G:149:LYS:HZ3	1.80	0.44
5:E:14:LYS:N	5:E:14:LYS:HE2	2.32	0.44
3:C:118:ARG:O	3:C:141:ILE:CG2	2.66	0.44
3:C:150:TRP:HZ3	3:C:171:ALA:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:MET:HG3	4:D:200:PHE:CD1	2.53	0.44
4:D:272:ASP:O	4:D:275:LYS:HB2	2.17	0.44
5:E:74:TYR:CE2	5:E:137:ARG:HA	2.53	0.44
4:D:141:ARG:HB2	4:D:154:VAL:O	2.18	0.43
5:E:93:LYS:HD3	5:E:93:LYS:HA	1.77	0.43
1:A:53:LYS:O	1:A:56:ASP:OD2	2.36	0.43
1:A:221:LEU:O	1:A:224:ALA:HB3	2.18	0.43
3:C:69:THR:O	3:C:76:ALA:HA	2.18	0.43
3:C:216:ARG:NH2	3:C:274:SER:HB2	2.33	0.43
5:E:121:ALA:O	5:E:122:ASN:CB	2.61	0.43
6:F:104:LEU:HA	6:F:104:LEU:HD23	1.75	0.43
1:A:104:GLU:O	1:A:108:HIS:HD2	2.01	0.43
5:E:5:HIS:NE2	5:E:61:LYS:HE3	2.33	0.43
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.53	0.43
1:A:11:ASP:OD2	1:A:11:ASP:C	2.61	0.43
4:D:84:LEU:HD23	4:D:85:VAL:H	1.84	0.43
5:E:62:ASN:C	5:E:64:ALA:N	2.74	0.43
6:F:60:LYS:HE3	6:F:112:TYR:CZ	2.53	0.43
1:A:64:ASP:O	1:A:66:ALA:N	2.52	0.43
1:A:120:PRO:HG3	2:B:201:GLY:O	2.18	0.43
1:A:151:ALA:O	1:A:154:THR:HG22	2.18	0.43
3:C:366:LEU:HB2	3:C:369:LEU:HB2	2.01	0.43
1:A:77:PRO:O	8:A:501:C69:H5	2.19	0.43
1:A:126:THR:OG1	8:A:501:C69:CAR	2.56	0.43
4:D:35:PHE:CE1	4:D:43:TYR:HB2	2.53	0.43
1:A:202:TYR:O	1:A:205:GLN:HB3	2.19	0.43
3:C:71:GLY:O	3:C:99:ALA:HB3	2.17	0.43
4:D:229:PRO:C	4:D:231:HIS:N	2.76	0.43
1:A:242:PHE:HZ	1:A:277:LEU:HD11	1.82	0.43
2:B:259:PHE:C	2:B:262:PRO:HD2	2.43	0.43
2:B:337:LEU:C	2:B:339:LYS:N	2.77	0.43
3:C:13:CYS:HA	3:C:331:GLN:HE22	1.82	0.43
5:E:97:THR:C	5:E:99:GLY:N	2.75	0.43
6:F:106:ARG:HG2	6:F:106:ARG:HH11	1.83	0.43
6:F:127:TYR:HB3	6:F:129:HIS:ND1	2.34	0.43
1:A:177:VAL:HG13	1:A:300:VAL:HG22	2.00	0.43
3:C:183:THR:CG2	3:C:185:TRP:H	2.09	0.43
4:D:270:THR:OG1	6:F:94:MET:HG2	2.19	0.43
5:E:91:GLY:C	5:E:93:LYS:H	2.25	0.43
6:F:25:PHE:CD2	6:F:26:SER:O	2.72	0.43
7:G:36:GLY:HA2	7:G:37:PRO:HD3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:HB2	1:A:175:THR:HG23	2.01	0.42
3:C:19:ASP:HB2	3:C:21:THR:HB	2.01	0.42
5:E:168:PHE:C	5:E:170:ASN:N	2.77	0.42
6:F:105:ARG:HG2	6:F:105:ARG:HH11	1.83	0.42
2:B:322:LYS:HG2	2:B:342:ILE:HD11	2.01	0.42
3:C:144:THR:OG1	6:F:28:GLN:NE2	2.32	0.42
4:D:255:ILE:O	4:D:259:LYS:HG3	2.19	0.42
5:E:10:ASP:C	5:E:12:ASP:N	2.76	0.42
6:F:101:PHE:O	6:F:104:LEU:HB2	2.19	0.42
7:G:27:GLU:OE2	7:G:27:GLU:HA	2.19	0.42
1:A:115:PRO:HD3	8:A:501:C69:H2	2.01	0.42
2:B:170:TYR:CZ	2:B:293:THR:HG22	2.55	0.42
2:B:180:ARG:HG3	2:B:180:ARG:HH11	1.83	0.42
2:B:198:LEU:HD12	2:B:203:ALA:HA	2.00	0.42
2:B:323:GLN:HB3	7:G:11:PHE:HD1	1.84	0.42
5:E:85:CYS:CB	5:E:90:GLN:NE2	2.82	0.42
5:E:150:ASP:O	5:E:152:GLN:N	2.52	0.42
1:A:280:GLU:O	1:A:280:GLU:HG3	2.19	0.42
1:A:309:ILE:HA	1:A:312:ARG:NE	2.34	0.42
2:B:302:VAL:CG2	2:B:347:PRO:HG3	2.49	0.42
4:D:76:LEU:HD23	4:D:76:LEU:HA	1.88	0.42
5:E:66:ARG:HG3	5:E:66:ARG:NH1	2.32	0.42
5:E:87:SER:OG	5:E:90:GLN:HB2	2.20	0.42
1:A:403:ILE:O	1:A:403:ILE:HG22	2.20	0.42
2:B:209:ASP:O	2:B:213:VAL:HG23	2.19	0.42
5:E:96:TYR:O	5:E:100:ILE:HG12	2.20	0.42
1:A:21:TYR:OH	1:A:101:LEU:O	2.31	0.42
1:A:295:PRO:O	1:A:298:GLU:N	2.49	0.42
1:A:305:GLN:C	1:A:307:CYS:H	2.28	0.42
2:B:170:TYR:O	2:B:172:GLY:N	2.52	0.42
6:F:130:LYS:O	6:F:133:ASP:N	2.50	0.42
1:A:4:ARG:HD2	4:D:62:LYS:HE2	2.00	0.42
1:A:311:VAL:O	1:A:311:VAL:HG13	2.20	0.42
2:B:279:ALA:HB3	2:B:320:GLU:HG2	1.97	0.42
2:B:316:ARG:HG2	2:B:316:ARG:HH11	1.84	0.42
2:B:322:LYS:HD2	7:G:16:VAL:CG1	2.50	0.42
3:C:173:ILE:HD11	3:C:191:PHE:CE1	2.54	0.42
3:C:228:LEU:C	3:C:228:LEU:HD23	2.45	0.42
4:D:146:TYR:HD1	4:D:147:ARG:HG3	1.85	0.42
4:D:258:SER:O	4:D:261:TYR:N	2.52	0.42
7:G:36:GLY:CA	7:G:63:PRO:HG3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TYR:CD1	1:A:137:PRO:HG2	2.55	0.42
3:C:10:PRO:CG	6:F:124:GLU:HG2	2.42	0.42
4:D:152:MET:HE3	4:D:154:VAL:CG2	2.50	0.42
7:G:79:VAL:HG11	7:G:109:TYR:HD1	1.83	0.42
1:A:79:ARG:HH11	1:A:79:ARG:CG	2.31	0.42
1:A:80:HIS:CE1	1:A:192:HIS:CE1	3.06	0.42
1:A:107:ASP:CG	4:D:147:ARG:HH22	2.25	0.42
2:B:194:ILE:C	2:B:196:LEU:N	2.78	0.42
4:D:80:TYR:CD2	4:D:95:LEU:HD22	2.54	0.42
4:D:199:LEU:HD12	4:D:199:LEU:N	2.34	0.42
5:E:14:LYS:HE2	5:E:14:LYS:CA	2.49	0.42
5:E:22:LEU:HD23	5:E:41:ILE:CB	2.50	0.42
5:E:78:CYS:O	5:E:82:LEU:HB2	2.19	0.42
2:B:294:ARG:O	2:B:295:SER:C	2.63	0.41
4:D:261:TYR:HE2	6:F:152:SER:OG	2.01	0.41
2:B:277:GLY:O	2:B:278:VAL:C	2.63	0.41
5:E:21:LEU:HD12	5:E:132:TYR:CD2	2.55	0.41
5:E:42:VAL:O	5:E:46:ILE:HG13	2.20	0.41
5:E:78:CYS:HB2	5:E:144:LEU:CD1	2.51	0.41
1:A:38:LYS:HG3	1:A:72:TYR:CD2	2.54	0.41
1:A:211:ARG:NH2	1:A:274:GLU:OE2	2.48	0.41
1:A:218:GLU:C	1:A:220:SER:N	2.77	0.41
2:B:194:ILE:C	2:B:196:LEU:H	2.28	0.41
3:C:96:ASN:C	3:C:97:ARG:HD3	2.43	0.41
3:C:130:ASP:CG	3:C:130:ASP:O	2.62	0.41
4:D:59:ILE:HG12	4:D:60:SER:N	2.34	0.41
1:A:155:SER:C	1:A:157:GLN:H	2.27	0.41
2:B:184:ILE:HD11	2:B:268:PRO:HB3	2.02	0.41
3:C:107:ASN:ND2	3:C:109:LYS:HB2	2.34	0.41
4:D:141:ARG:HB3	4:D:155:GLU:CB	2.50	0.41
4:D:161:VAL:HG21	4:D:232:THR:HG21	2.02	0.41
7:G:99:ASP:O	7:G:102:GLY:N	2.52	0.41
1:A:122:ASN:HD22	1:A:122:ASN:HA	1.70	0.41
1:A:195:ILE:HG22	1:A:282:PHE:CE1	2.55	0.41
1:A:273:TYR:HB3	1:A:277:LEU:HD12	2.02	0.41
2:B:163:VAL:HG22	2:B:164:THR:H	1.85	0.41
2:B:283:PHE:HB2	2:B:324:LEU:HD12	2.02	0.41
2:B:326:LEU:O	2:B:326:LEU:HG	2.20	0.41
4:D:75:LEU:HD23	4:D:75:LEU:O	2.20	0.41
4:D:184:GLU:OE1	6:F:158:ARG:CB	2.67	0.41
5:E:16:ILE:CG1	5:E:129:MET:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:C	1:A:93:MET:N	2.78	0.41
1:A:385:ALA:HA	1:A:390:PHE:CG	2.55	0.41
6:F:90:PHE:CD1	6:F:94:MET:HE2	2.56	0.41
1:A:14:THR:HG22	1:A:15:GLY:N	2.34	0.41
1:A:153:TRP:NE1	1:A:162:THR:H	2.18	0.41
1:A:263:SER:O	1:A:264:LYS:C	2.63	0.41
3:C:6:PHE:CE2	3:C:35:TYR:CG	3.08	0.41
3:C:112:ALA:HB1	3:C:148:LEU:HD13	2.03	0.41
6:F:40:VAL:HG23	6:F:41:ARG:N	2.35	0.41
1:A:349:LEU:C	1:A:351:GLU:N	2.78	0.41
2:B:169:VAL:HG13	2:B:173:PHE:O	2.21	0.41
2:B:266:PHE:CE1	2:B:316:ARG:HG3	2.55	0.41
3:C:16:TRP:NE1	3:C:335:LEU:HD21	2.36	0.41
4:D:230:ARG:HD3	4:D:231:HIS:CE1	2.56	0.41
4:D:277:LEU:O	4:D:279:ARG:N	2.54	0.41
6:F:76:VAL:N	6:F:113:ASP:OD2	2.54	0.41
6:F:108:PRO:HB3	6:F:112:TYR:O	2.20	0.41
1:A:52:MET:HE2	1:A:56:ASP:CB	2.40	0.41
1:A:262:ILE:C	1:A:264:LYS:H	2.29	0.41
2:B:259:PHE:C	2:B:259:PHE:CD2	2.98	0.41
3:C:155:VAL:HG21	3:C:180:PRO:HG3	2.03	0.41
3:C:185:TRP:CZ2	3:C:231:ALA:HB2	2.56	0.41
3:C:326:LYS:HA	3:C:326:LYS:HD3	1.78	0.41
3:C:345:PHE:CD1	3:C:345:PHE:C	2.98	0.41
4:D:184:GLU:OE1	6:F:158:ARG:NE	2.41	0.41
5:E:58:TYR:CD2	5:E:69:ILE:HD11	2.55	0.41
5:E:76:SER:O	5:E:80:LYS:HG3	2.20	0.41
5:E:100:ILE:HA	5:E:134:GLN:NE2	2.27	0.41
5:E:139:GLU:C	5:E:141:GLY:N	2.78	0.41
6:F:8:TYR:HE2	6:F:139:MET:CE	2.33	0.41
6:F:52:THR:O	7:G:114:PHE:CD1	2.74	0.41
7:G:114:PHE:HD2	7:G:114:PHE:HA	1.78	0.41
2:B:241:VAL:HA	2:B:254:VAL:O	2.21	0.41
3:C:14:HIS:HA	3:C:24:ALA:O	2.22	0.41
4:D:43:TYR:CE2	4:D:59:ILE:HG13	2.56	0.41
5:E:105:ILE:HB	5:E:106:PRO:CD	2.51	0.41
5:E:108:GLU:HA	5:E:109:PRO:HD3	1.81	0.41
6:F:14:ALA:O	6:F:17:GLN:HB3	2.21	0.41
1:A:174:VAL:HG12	1:A:175:THR:H	1.86	0.40
1:A:174:VAL:HG12	1:A:175:THR:N	2.36	0.40
1:A:202:TYR:N	1:A:202:TYR:CD2	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HH11	5:E:159:TRP:HZ3	1.67	0.40
1:A:340:LYS:HE3	1:A:340:LYS:HB3	1.96	0.40
1:A:393:VAL:HG21	1:A:414:PHE:CG	2.55	0.40
3:C:118:ARG:HG3	3:C:118:ARG:NH1	2.34	0.40
4:D:176:VAL:HG21	6:F:85:ILE:HG21	2.03	0.40
4:D:276:VAL:O	4:D:277:LEU:C	2.64	0.40
5:E:156:PRO:O	5:E:157:SER:C	2.64	0.40
7:G:99:ASP:OD2	7:G:101:ASN:HB2	2.21	0.40
1:A:120:PRO:CG	2:B:201:GLY:HA3	2.51	0.40
1:A:201:THR:O	1:A:202:TYR:C	2.64	0.40
1:A:254:LYS:HE2	1:A:275:ARG:CZ	2.51	0.40
1:A:292:PHE:O	1:A:293:THR:HG23	2.21	0.40
3:C:266:PHE:CD1	3:C:266:PHE:O	2.73	0.40
7:G:91:ILE:HD13	7:G:128:TRP:CD1	2.57	0.40
3:C:132:TRP:C	3:C:133:VAL:HG13	2.46	0.40
3:C:183:THR:C	3:C:185:TRP:N	2.80	0.40
3:C:183:THR:CB	3:C:189:MET:HE1	2.45	0.40
4:D:64:TYR:CB	4:D:92:ASN:HD22	2.29	0.40
4:D:64:TYR:O	4:D:65:LYS:C	2.65	0.40
4:D:277:LEU:HD12	6:F:102:PHE:HE1	1.86	0.40
6:F:105:ARG:NH1	6:F:105:ARG:HG2	2.36	0.40
3:C:14:HIS:O	3:C:331:GLN:OE1	2.39	0.40
3:C:160:GLY:HA3	3:C:205:VAL:HG12	2.03	0.40
4:D:1:MET:HE3	4:D:4:LEU:HD23	2.03	0.40
5:E:150:ASP:O	5:E:151:PRO:C	2.65	0.40
6:F:53:ILE:HD12	6:F:53:ILE:H	1.85	0.40
1:A:83:VAL:HG22	1:A:84:GLU:N	2.36	0.40
1:A:349:LEU:C	1:A:351:GLU:H	2.28	0.40
2:B:321:LEU:C	2:B:323:GLN:N	2.78	0.40
3:C:56:THR:OG1	3:C:70:CYS:O	2.38	0.40
3:C:144:THR:H	6:F:28:GLN:NE2	2.19	0.40
4:D:280:ALA:HA	6:F:130:LYS:HD3	2.03	0.40
6:F:138:PHE:CE2	6:F:142:ILE:HG21	2.57	0.40
7:G:119:ASP:C	7:G:121:SER:N	2.80	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	393/418 (94%)	317 (81%)	61 (16%)	15 (4%)	2	4
2	B	193/394 (49%)	150 (78%)	36 (19%)	7 (4%)	2	4
3	C	337/372 (91%)	302 (90%)	31 (9%)	4 (1%)	10	20
4	D	273/300 (91%)	219 (80%)	41 (15%)	13 (5%)	2	2
5	E	171/178 (96%)	141 (82%)	24 (14%)	6 (4%)	3	5
6	F	164/168 (98%)	146 (89%)	16 (10%)	2 (1%)	10	20
7	G	132/151 (87%)	109 (83%)	21 (16%)	2 (2%)	8	15
All	All	1663/1981 (84%)	1384 (83%)	230 (14%)	49 (3%)	3	6

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
2	B	171	GLU
2	B	278	VAL
4	D	203	ARG
4	D	215	ALA
4	D	237	ARG
5	E	153	ASN
1	A	59	ASP
1	A	65	GLU
1	A	70	PRO
1	A	145	ALA
3	C	203	GLY
3	C	338	GLY
4	D	38	PHE
4	D	138	GLY
4	D	170	LYS
4	D	278	ASN
5	E	122	ASN

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Mol	Chain	Res	Type
1	A	77	PRO
1	A	144	GLN
1	A	296	ILE
3	C	50	GLU
4	D	174	ASP
4	D	230	ARG
5	E	87	SER
5	E	158	LYS
6	F	110	GLU
1	A	186	ILE
1	A	264	LYS
2	B	172	GLY
4	D	140	ASN
4	D	244	ILE
4	D	277	LEU
1	A	217	PRO
1	A	293	THR
1	A	393	VAL
2	B	336	LYS
3	C	320	GLY
5	E	146	GLU
7	G	40	GLY
2	B	184	ILE
6	F	102	PHE
1	A	216	PRO
1	A	360	PRO
2	B	256	GLY
2	B	311	PRO
5	E	11	PRO
4	D	103	PRO
7	G	64	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/363 (96%)	332 (95%)	17 (5%)	22	43
2	B	163/345 (47%)	147 (90%)	16 (10%)	7	15
3	C	286/313 (91%)	271 (95%)	15 (5%)	21	39
4	D	239/264 (90%)	226 (95%)	13 (5%)	20	38
5	E	154/159 (97%)	146 (95%)	8 (5%)	21	39
6	F	153/155 (99%)	140 (92%)	13 (8%)	10	18
7	G	88/123 (72%)	85 (97%)	3 (3%)	32	57
All	All	1432/1722 (83%)	1347 (94%)	85 (6%)	18	33

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	14	THR
1	A	19	LEU
1	A	70	PRO
1	A	84	GLU
1	A	88	LEU
1	A	143	VAL
1	A	217	PRO
1	A	230	ARG
1	A	255	GLN
1	A	257	THR
1	A	297	SER
1	A	335	LEU
1	A	363	ILE
1	A	405	PRO
1	A	406	SER
1	A	407	ILE
2	B	155	VAL
2	B	175	LEU
2	B	176	PRO
2	B	182	LEU
2	B	200	ARG
2	B	220	LEU
2	B	252	ILE
2	B	274	GLU
2	B	276	VAL

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Mol	Chain	Res	Type
2	B	281	LEU
2	B	303	LEU
2	B	311	PRO
2	B	322	LYS
2	B	326	LEU
2	B	337	LEU
2	B	342	ILE
3	C	5	SER
3	C	7	LEU
3	C	8	VAL
3	C	21	THR
3	C	30	HIS
3	C	56	THR
3	C	106	PRO
3	C	107	ASN
3	C	131	TRP
3	C	183	THR
3	C	187	SER
3	C	210	PHE
3	C	321	LEU
3	C	346	CYS
3	C	368	ASP
4	D	9	ARG
4	D	58	SER
4	D	65	LYS
4	D	84	LEU
4	D	115	MET
4	D	116	LEU
4	D	140	ASN
4	D	160	ARG
4	D	204	GLU
4	D	229	PRO
4	D	258	SER
4	D	270	THR
4	D	274	LEU
5	E	22	LEU
5	E	38	ASP
5	E	63	GLU
5	E	67	THR
5	E	82	LEU
5	E	95	MET
5	E	133	LEU

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Mol	Chain	Res	Type
5	E	144	LEU
6	F	20	LEU
6	F	22	LEU
6	F	53	ILE
6	F	66	SER
6	F	70	VAL
6	F	72	VAL
6	F	85	ILE
6	F	102	PHE
6	F	104	LEU
6	F	128	LYS
6	F	152	SER
6	F	160	VAL
6	F	165	LEU
7	G	15	ASP
7	G	29	ASP
7	G	114	PHE

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

Mol	Chain	Res	Type
1	A	80	HIS
1	A	122	ASN
1	A	157	GLN
1	A	176	HIS
1	A	192	HIS
1	A	206	GLN
1	A	243	ASN
1	A	255	GLN
1	A	289	ASN
1	A	306	ASN
1	A	318	ASN
1	A	366	GLN
1	A	395	HIS
1	A	411	ASN
2	B	231	GLN
2	B	267	GLN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	4	HIS
3	C	33	HIS

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Mol	Chain	Res	Type
3	C	44	GLN
3	C	46	HIS
3	C	65	ASN
3	C	107	ASN
3	C	325	HIS
3	C	331	GLN
4	D	49	ASN
4	D	92	ASN
4	D	140	ASN
4	D	197	GLN
4	D	202	HIS
4	D	231	HIS
5	E	62	ASN
5	E	83	GLN
5	E	102	ASN
5	E	134	GLN
5	E	152	GLN
5	E	167	GLN
5	E	170	ASN
6	F	28	GLN
6	F	34	ASN
6	F	78	GLN
7	G	50	ASN
7	G	65	ASN
7	G	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	C69	A	501	-	25,25,25	1.88	3 (12%)	33,35,35	2.55	8 (24%)

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
8	C69	A	501	-	-	8/12/25/25	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	501	C69	CAE-NAF	-7.92	1.33	1.43
8	A	501	C69	CAQ-NAF	-3.36	1.33	1.37
8	A	501	C69	CAR-CAQ	2.03	1.53	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	501	C69	CAQ-CAR-SAS	-7.74	100.94	107.61
8	A	501	C69	CAR-CAQ-NAF	7.24	116.99	112.14
8	A	501	C69	CAB-OAA-CAD	-5.31	109.73	117.51
8	A	501	C69	CAL-OAM-CAN	-4.36	108.15	117.50
8	A	501	C69	OAW-CAQ-NAF	-3.55	122.36	125.12
8	A	501	C69	OAA-CAD-CAE	3.23	120.05	116.04
8	A	501	C69	OAA-CAD-CAC	-3.06	118.80	124.08
8	A	501	C69	CAH-CAG-NAF	-2.09	111.29	113.54

There are no chirality outliers.

All (8) torsion outliers are listed below:

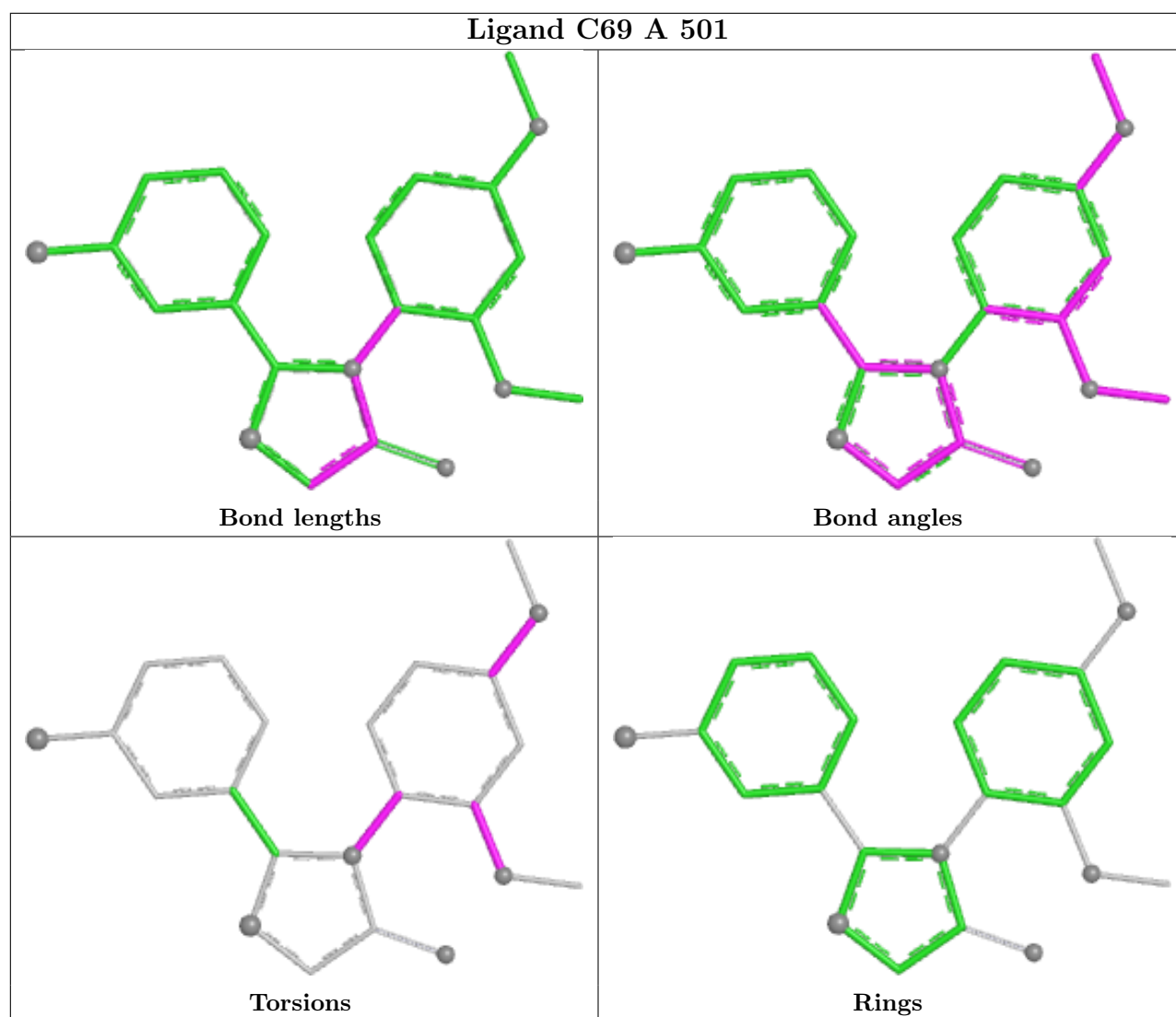
Mol	Chain	Res	Type	Atoms
8	A	501	C69	CAD-CAE-NAF-CAQ
8	A	501	C69	CAD-CAE-NAF-CAG
8	A	501	C69	CAP-CAE-NAF-CAG
8	A	501	C69	CAC-CAN-OAM-CAL
8	A	501	C69	CAO-CAN-OAM-CAL
8	A	501	C69	CAE-CAD-OAA-CAB
8	A	501	C69	CAC-CAD-OAA-CAB
8	A	501	C69	CAP-CAE-NAF-CAQ

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	501	C69	11	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/418 (95%)	0.15	8 (2%) 65 63	28, 60, 92, 107	0
2	B	195/394 (49%)	0.54	11 (5%) 30 30	35, 73, 109, 115	0
3	C	341/372 (91%)	0.01	4 (1%) 76 76	32, 52, 78, 95	0
4	D	277/300 (92%)	0.18	6 (2%) 62 60	30, 60, 96, 114	0
5	E	173/178 (97%)	0.47	6 (3%) 47 44	52, 79, 111, 119	0
6	F	166/168 (98%)	-0.04	1 (0%) 85 86	28, 56, 74, 87	0
7	G	138/151 (91%)	0.91	17 (12%) 8 6	49, 100, 118, 120	0
All	All	1689/1981 (85%)	0.25	53 (3%) 51 49	28, 63, 105, 120	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	85	CYS	4.6
7	G	38	ASP	4.6
7	G	45	CYS	4.3
7	G	52	THR	4.2
4	D	215	ALA	3.7
7	G	47	ARG	3.7
2	B	348	PRO	3.6
1	A	82	ILE	3.6
7	G	46	LEU	3.5
3	C	201	SER	3.3
1	A	416	VAL	3.3
6	F	3	ALA	3.3
5	E	154	ASP	3.1
1	A	156	ARG	3.1
7	G	41	GLU	3.0
2	B	183	ASP	3.0
7	G	35	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	2.9
7	G	48	GLN	2.8
2	B	174	SER	2.8
7	G	22	ASN	2.8
7	G	83	LEU	2.8
4	D	136	LYS	2.7
1	A	161	ARG	2.7
2	B	347	PRO	2.7
5	E	110	GLY	2.7
7	G	43	ASP	2.7
1	A	2	ALA	2.6
3	C	29	ASN	2.6
5	E	88	LYS	2.5
1	A	158	VAL	2.5
2	B	291	ILE	2.5
7	G	50	ASN	2.5
4	D	282	PRO	2.5
4	D	228	PHE	2.4
7	G	49	GLY	2.4
2	B	333	ASP	2.3
1	A	52	MET	2.3
7	G	93	LYS	2.3
7	G	44	SER	2.3
2	B	162	GLY	2.3
3	C	372	VAL	2.3
3	C	142	ARG	2.3
5	E	153	ASN	2.2
7	G	9	ALA	2.2
2	B	286	ILE	2.2
4	D	203	ARG	2.1
2	B	170	TYR	2.1
7	G	128	TRP	2.1
4	D	206	PRO	2.1
5	E	156	PRO	2.1
2	B	329	VAL	2.0
2	B	325	TYR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

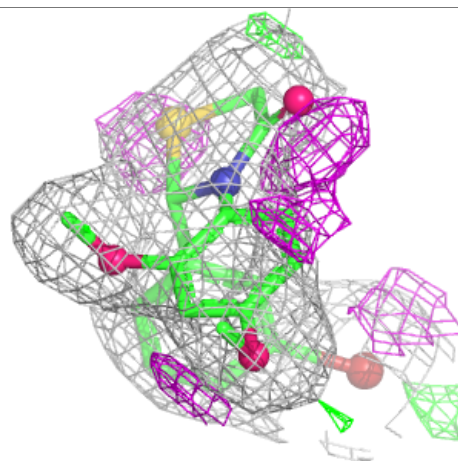
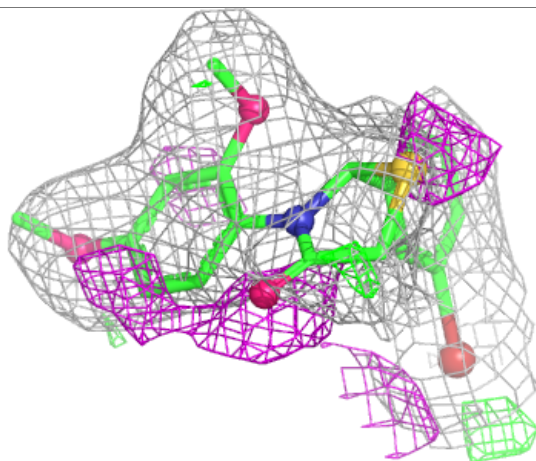
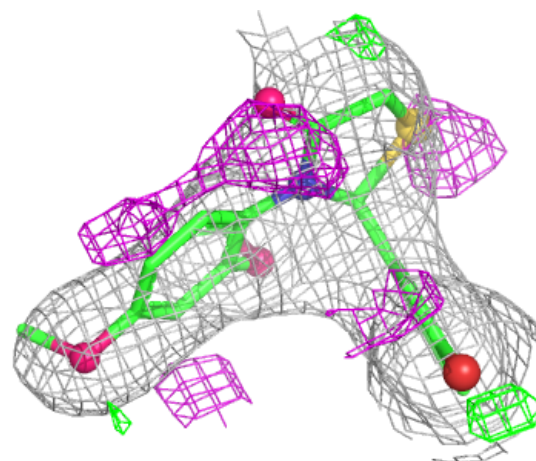
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
8	C69	A	501	23/23	0.92	0.15	71,75,83,85	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 C69 A 501:

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.