Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:44 pm BST

PDB ID	:	3UKU
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 following versions of software and data (see references ⓘ) were used in the production of this report:

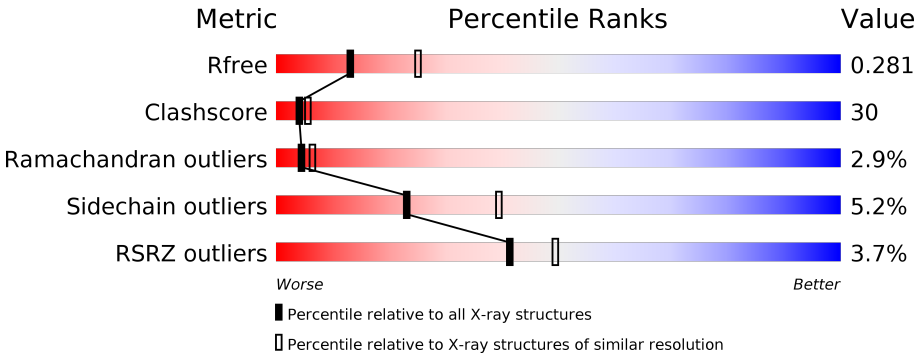
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 49% 41% 5% 5%
2	B	394	6% 23% 22% 51%
3	C	372	50% 40% 8%
4	D	300	% 47% 40% 5% 8%
5	E	178	4% 39% 54%
6	F	168	% 53% 42%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G	151	7% 56% 34% 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			

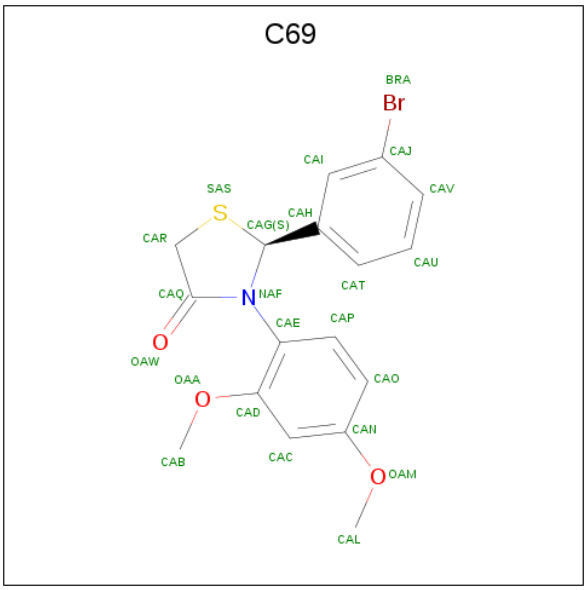
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

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 (three-letter code: C69) (formula: $C_{17}H_{16}BrNO_3S$).



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		

Continued on next page...

Continued from previous page...

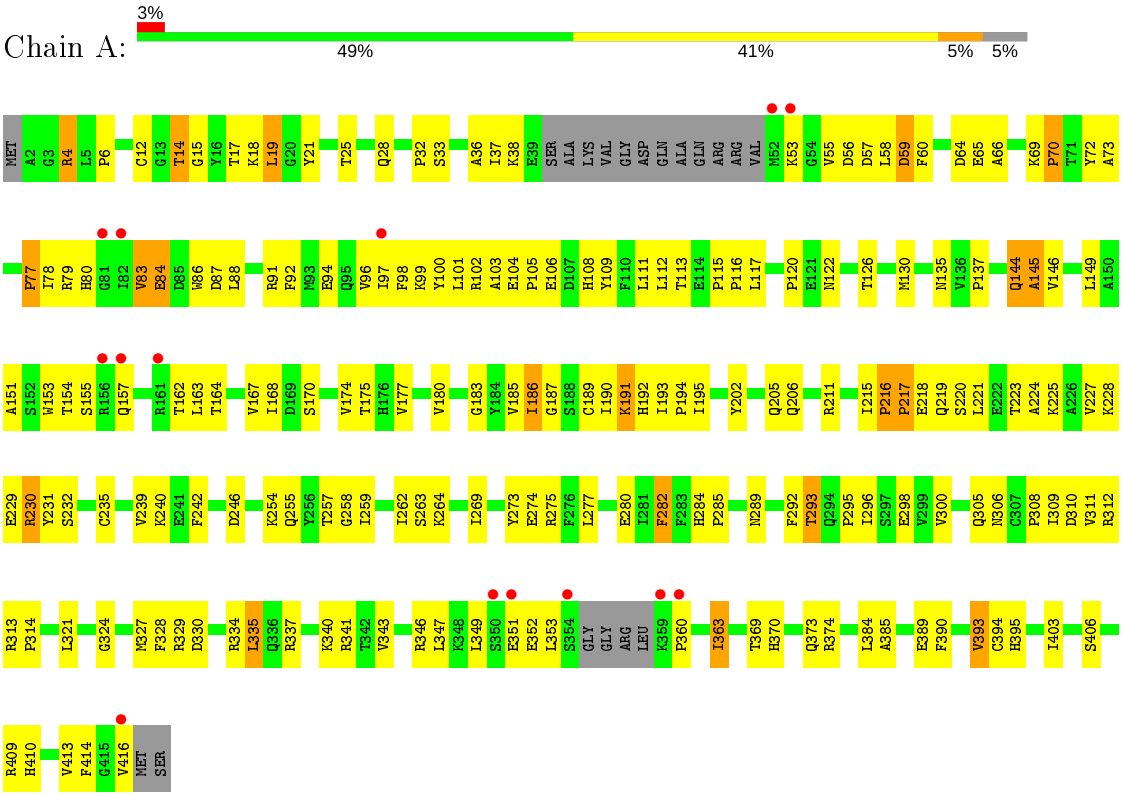
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	6	Total O 6 6	0	0
9	F	15	Total O 15 15	0	0
9	G	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

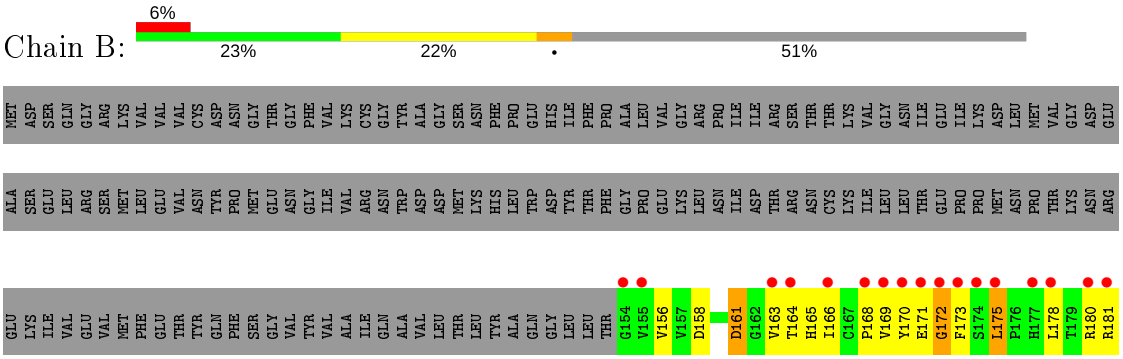
- Molecule 1: ACTIN-LIKE PROTEIN 3

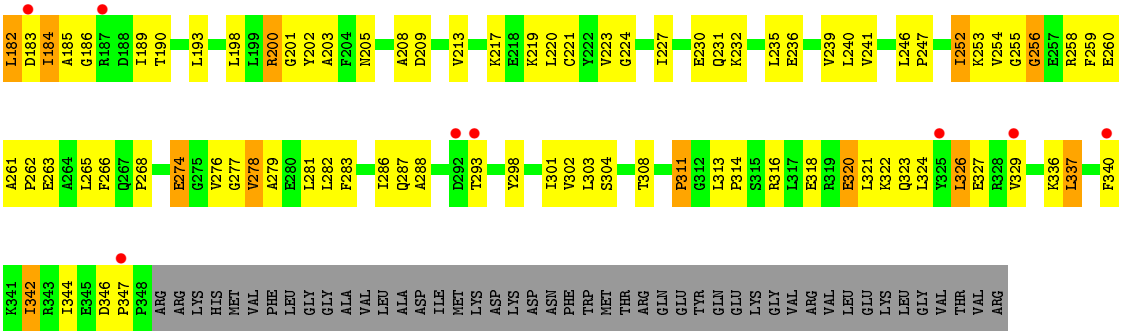
Chain A:



- Molecule 2: ACTIN-LIKE PROTEIN 2

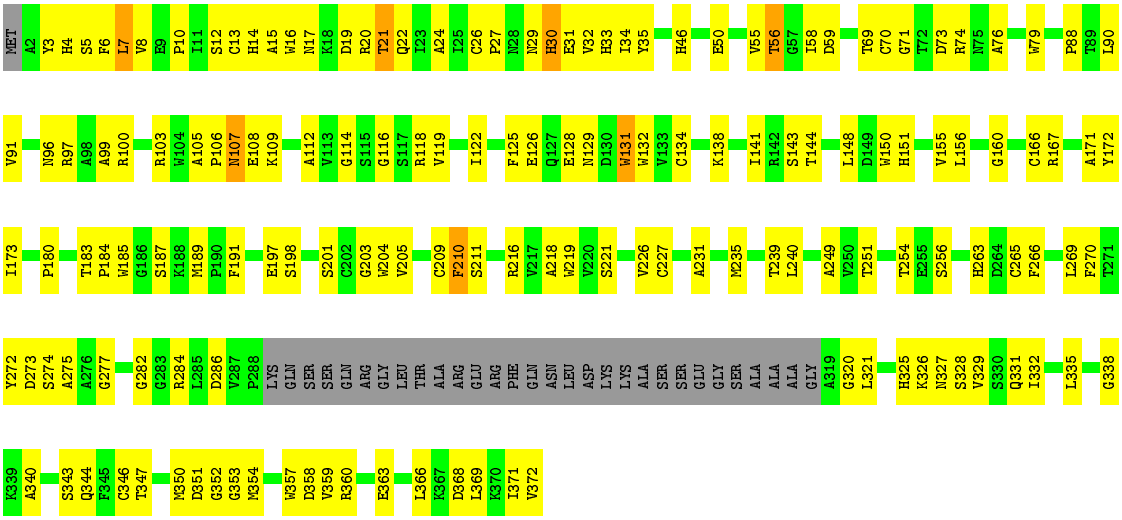
Chain B:





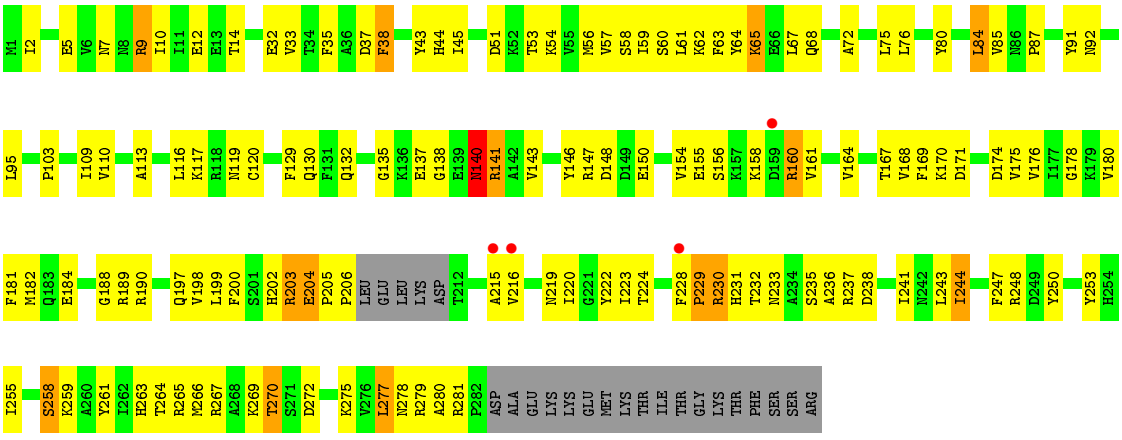
• Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C:



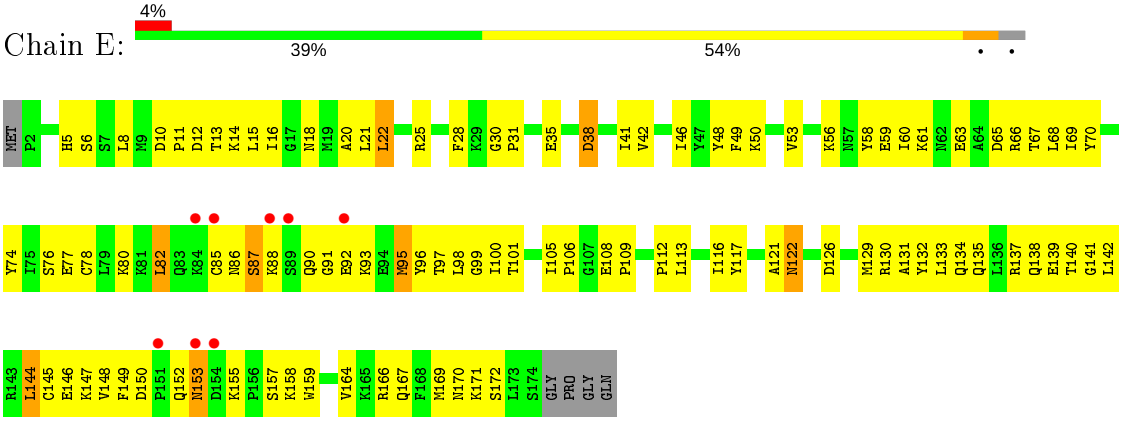
• Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:



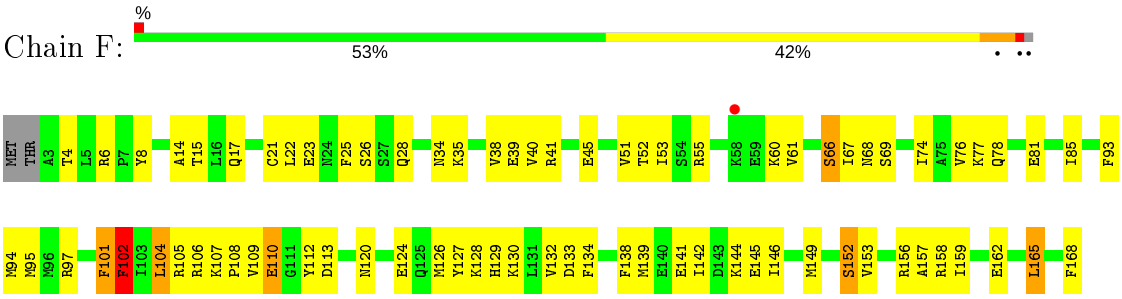
• Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:



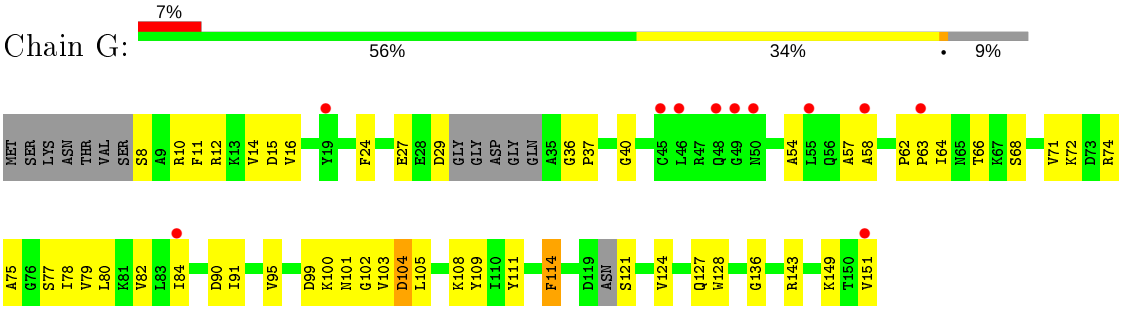
- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:



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

Chain G:



4 Data and refinement statistics (i)

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 43.51 – 2.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.75) 90.6 (43.51-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.301 0.239 , 0.281	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 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.42	0/3278	0.66	0/4447
2	B	0.40	0/1557	0.64	0/2110
3	C	0.47	0/2702	0.73	0/3673
4	D	0.42	0/2265	0.66	0/3062
5	E	0.34	0/1437	0.60	0/1940
6	F	0.46	0/1386	0.70	0/1858
7	G	0.33	0/982	0.56	0/1330
All	All	0.42	0/13607	0.66	0/18420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3197	0	3145	188	0
2	B	1528	0	1530	107	0
3	C	2633	0	2560	151	0
4	D	2217	0	2158	149	0
5	E	1403	0	1398	108	0
6	F	1364	0	1403	101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	971	0	895	54	0
8	A	23	0	16	11	0
9	A	25	0	0	1	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	787	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 30.

All (787) 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
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:371:ILE:HG22	3:C:372:VAL:HG23	1.47	0.96
3:C:74:ARG:HG2	3:C:97:ARG:O	1.66	0.96
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:H	1:A:363:ILE:HD13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:LEU:HD11	2:B:278:VAL:N	1.92	0.83
3:C:96:ASN:O	3:C:97:ARG:HD3	1.78	0.82
1:A:206:GLN:HE21	5:E:166:ARG:HH22	1.27	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:254:THR:HA	3:C:340:ALA:O	1.80	0.80
3:C:32:VAL:HG22	3:C:58:ILE:HD11	1.64	0.80
1:A:206:GLN:HE21	5:E:166:ARG:NH2	1.81	0.79
4:D:168:VAL:HG22	4:D:220:ILE:HG12	1.62	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:228:LYS:HA	1:A:232:SER:OG	1.87	0.74
3:C:107:ASN:HD22	3:C:107:ASN:C	1.88	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
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
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:HA	2:B:274:GLU:OE1	1.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:A:18:LYS:N	2.06	0.71
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
1:A:111:LEU:HD23	1:A:111:LEU:C	2.12	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:313:ARG:HB2	1:A:314:PRO:HD3	1.74	0.69
1:A:55:VAL:CG1	1:A:58:LEU:HD12	2.22	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:205:PRO:HB3	4:D:222:TYR:CE2	2.27	0.69
4:D:64:TYR:HB3	4:D:92:ASN:ND2	2.07	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
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.09	0.68
1:A:246:ASP:OD1	5:E:50:LYS:HE3	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	2:B:175:LEU:HD23	2.10	0.67
3:C:107:ASN:HD22	3:C:108:GLU:N	1.93	0.67
4:D:59:ILE:O	4:D:91:TYR:HB3	1.95	0.67
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:109:LYS:H	1.41	0.66
5:E:65:ASP:O	5:E:69:ILE:HG13	1.94	0.66
6:F:128:LYS:O	6:F:132:VAL:HG23	1.94	0.66
6:F:38:VAL:HB	6:F:66:SER:HB3	1.77	0.66
2:B:193:LEU:HD23	2:B:213:VAL:HG12	1.76	0.66
1:A:363:ILE:CD1	1:A:363:ILE:H	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
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:O	1:A:55:VAL:HG12	1.98	0.64
1:A:112:LEU:HD11	1:A:130:MET:CE	2.27	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:160:ARG:HH11	4:D:160:ARG:HB3	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:261:TYR:HE2	6:F:152:SER:HG	1.45	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
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
1:A:327:MET:HE2	1:A:374:ARG:HB2	1.79	0.62
3:C:183:THR:HB	3:C:189:MET:CE	2.29	0.62
1:A:327:MET:CE	1:A:374:ARG:HB2	2.30	0.62
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
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
5:E:16:ILE:O	5:E:16:ILE:HG23	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:ND2	4:D:140:ASN:H	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
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:79:VAL:HG21	7:G:109:TYR:CD1	2.36	0.60
3:C:116:GLY:C	3:C:118:ARG:H	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:LEU:O	5:E:98:LEU:HD13	2.02	0.60
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.01	0.60
3:C:90:LEU:HD23	3:C:91:VAL:N	2.17	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
5:E:145:CYS:C	5:E:147:LYS:H	2.05	0.59
1:A:19:LEU:CD1	1:A:96:VAL:HG13	2.31	0.59
1:A:25:THR:HG22	1:A:25:THR:O	2.01	0.59
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.17	0.59
5:E:152:GLN:HB3	5:E:155:LYS:HZ1	1.67	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
7:G:103:VAL:HG11	7:G:136:GLY:CA	2.33	0.59
1:A:262:ILE:HG22	1:A:263:SER:N	2.17	0.59
1:A:12:CYS:HB3	1:A:78:ILE:HD13	1.85	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: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
3:C:183:THR:HB	3:C:189:MET:HE3	1.84	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:230:ARG:CB	1:A:230:ARG:HH11	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:N	1:A:363:ILE:HD13	2.14	0.57
4:D:135:GLY:O	4:D:137:GLU:HG3	2.04	0.57
6:F:146:ILE:HA	6:F:149:MET:CE	2.34	0.57
8:A:501:C69:CAG	8:A:501:C69:OAA	2.52	0.57
3:C:118:ARG:HG3	3:C:118:ARG:HH11	1.68	0.57
3:C:19:ASP:O	3:C:20:ARG:HB2	2.03	0.57
4:D:233:ASN:OD1	4:D:235:SER:N	2.37	0.57
4:D:91:TYR:CD1	4:D:91:TYR:N	2.72	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
4:D:158:LYS:HD3	4:D:158:LYS:C	2.25	0.57
1:A:352:GLU:C	1:A:353:LEU:HD22	2.24	0.57
3:C:107:ASN:C	3:C:107:ASN:ND2	2.58	0.57
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.40	0.57
6:F:60:LYS:HE3	6:F:112:TYR:CE2	2.39	0.57
3:C:105:ALA:HA	3:C:150:TRP:CD1	2.40	0.57
4:D:65:LYS:H	4:D:65:LYS:HE2	1.68	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:H	4:D:223:ILE:HD12	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:CD1	3:C:357:TRP:N	2.73	0.56
4:D:65:LYS:HZ2	4:D:65:LYS:HB3	1.69	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
4:D:198:VAL:C	4:D:199:LEU:HD12	2.25	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:HE2	1.87	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
7:G:8:SER:C	7:G:10:ARG:H	2.07	0.56
1:A:190:ILE:O	1:A:191:LYS:HD2	2.06	0.55
3:C:327:ASN:H	3:C:351:ASP:HB3	1.71	0.55
4:D:267:ARG:HH11	4:D:267:ARG:HG3	1.72	0.55
1:A:211:ARG:NH1	5:E:159:TRP:CZ3	2.74	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:131:TRP:O	3:C:131:TRP:HE3	1.89	0.55
3:C:114:GLY:H	3:C:148:LEU:HD11	1.71	0.55
4:D:147:ARG:HD3	4:D:150:GLU:OE2	2.06	0.55
1:A:87:ASP:CG	4:D:264:THR:HG22	2.27	0.55
1:A:185:VAL:O	1:A:187:GLY:N	2.37	0.55
1:A:194:PRO:C	1:A:195:ILE:HD12	2.27	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
4:D:265:ARG:HG2	4:D:265:ARG:NH1	2.22	0.55
4:D:59:ILE:HD13	4:D:61:LEU:HD11	1.88	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
4:D:223:ILE:HG21	4:D:247:PHE:CE2	2.41	0.55
4:D:265:ARG:HH11	4:D:265:ARG:HG2	1.71	0.55
3:C:97:ARG:NE	6:F:28:GLN:O	2.30	0.55
6:F:53:ILE:HA	7:G:114:PHE:CD1	2.41	0.55
1:A:17:THR:HG1	1:A:92:PHE:HZ	1.55	0.55
2:B:298:TYR:CD1	2:B:340:PHE:HE1	2.24	0.55
1:A:274:GLU:OE1	1:A:274:GLU:N	2.40	0.54
1:A:69:LYS:HB3	1:A:72:TYR:HB2	1.88	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:343:VAL:HG22	1:A:363:ILE:HG13	1.89	0.54
1:A:80:HIS:HE1	1:A:192:HIS:CE1	2.25	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
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:NH1	4:D:9:ARG:HG2	2.23	0.54
1:A:211:ARG:NH1	5:E:159:TRP:HZ3	2.05	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
4:D:147:ARG:HD3	4:D:150:GLU:CD	2.27	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:79:VAL:HG11	7:G:109:TYR:CD1	2.43	0.54
1:A:112:LEU:HD11	1:A:130:MET:HE3	1.90	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
5:E:157:SER:C	5:E:159:TRP:H	2.11	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
1:A:308:PRO:HG3	2:B:208:ALA:HB2	1.90	0.53
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.74	0.53
3:C:122:ILE:O	3:C:134:CYS:HB2	2.09	0.53
3:C:14:HIS:N	3:C:331:GLN:HE22	2.03	0.53
1:A:87:ASP:OD2	4:D:264:THR:HG22	2.08	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:HD23	2:B:281:LEU:O	2.08	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:64:ASP:C	1:A:66:ALA:H	2.11	0.53
2:B:329:VAL:O	2:B:329:VAL:HG12	2.08	0.53
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:O	4:D:158:LYS:HD3	2.10	0.52
1:A:337:ARG:HD2	1:A:341:ARG:NH2	2.24	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:37:ILE:HD12	1:A:37:ILE:C	2.30	0.52
1:A:55:VAL:HG23	6:F:159:ILE:HD12	1.91	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:143:VAL:HG12	4:D:143:VAL:O	2.08	0.52
4:D:80:TYR:OH	4:D:119:ASN:ND2	2.37	0.52
1:A:334:ARG:HG2	1:A:334:ARG:HH11	1.74	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:O	1:A:393:VAL:HG23	2.10	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
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
4:D:10:ILE:O	4:D:14:THR:OG1	2.21	0.51
4:D:202:HIS:O	4:D:204:GLU:N	2.36	0.51
2:B:189:ILE:HG23	2:B:261:ALA:O	2.11	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:225:LYS:O	1:A:229:GLU:HG3	2.10	0.51
1:A:37:ILE:HB	9:A:611:HOH:O	2.10	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
5:E:97:THR:O	5:E:101:THR:HG23	2.10	0.51
5:E:6:SER:HB2	5:E:68:LEU:HD22	1.91	0.51
8:A:501:C69:CAP	8:A:501:C69:OAW	2.58	0.51
3:C:131:TRP:O	3:C:131:TRP:CE3	2.63	0.51
3:C:29:ASN:OD1	3:C:31:GLU:N	2.43	0.51
2:B:277:GLY:O	2:B:279:ALA:N	2.44	0.51
4:D:132:GLN:HB2	4:D:156:SER:OG	2.11	0.51
4:D:160:ARG:NH1	4:D:160:ARG:HB3	2.25	0.51
4:D:5:GLU:OE1	4:D:9:ARG:NE	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:132:TYR:CG	5:E:132:TYR:O	2.63	0.50
5:E:85:CYS:SG	5:E:149:PHE:HZ	2.34	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
5:E:99:GLY:O	5:E:134:GLN:HG3	2.11	0.50
6:F:141:GLU:HA	6:F:141:GLU:OE1	2.10	0.50
1:A:79:ARG:HH11	1:A:79:ARG:HG3	1.75	0.50
2:B:231:GLN:NE2	2:B:231:GLN:HA	2.27	0.50
3:C:27:PRO:C	3:C:29:ASN:H	2.15	0.50
3:C:15:ALA:CB	3:C:58:ILE:HG22	2.41	0.50
7:G:66:THR:O	7:G:72:LYS:HE3	2.12	0.50
3:C:7:LEU:O	3:C:352:GLY:HA3	2.12	0.49
4:D:248:ARG:C	4:D:248:ARG:HD3	2.32	0.49
6:F:109:VAL:O	6:F:110:GLU:C	2.50	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
3:C:27:PRO:C	3:C:29:ASN:N	2.66	0.49
5:E:5:HIS:HD2	5:E:65:ASP:OD2	1.96	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
1:A:104:GLU:OE1	1:A:105:PRO:CD	2.61	0.49
1:A:116:PRO:O	1:A:117:LEU:HB2	2.13	0.49
6:F:38:VAL:HG12	6:F:69:SER:OG	2.12	0.49
2:B:231:GLN:HE21	2:B:231:GLN:HA	1.77	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:HA	1:A:305:GLN:OE1	2.13	0.48
1:A:384:LEU:O	1:A:390:PHE: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:218:GLU:C	1:A:220:SER:H	2.16	0.48
1:A:231:TYR:CD1	1:A:254:LYS:HG3	2.49	0.48
1:A:25:THR:CG2	1:A:25:THR:O	2.62	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:10:ASP:C	5:E:12:ASP:H	2.15	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:243:LEU:HD12	6:F:168:PHE:CD1	2.49	0.47
4:D:35:PHE:CE1	4:D:43:TYR:CD1	3.02	0.47
2:B:308:THR:O	2:B:313:LEU:HD23	2.14	0.47
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
1:A:215:ILE:HD11	1:A:269:ILE:HG21	1.96	0.47
1:A:15:GLY:O	1:A:32:PRO:HA	2.15	0.47
4:D:61:LEU:HD23	4:D:63:PHE:CZ	2.49	0.47
3:C:100:ARG:NH2	6:F:23:GLU:OE2	2.47	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:157:GLN:HE22	1:A:369:THR:H	1.63	0.47
1:A:69:LYS:HD2	1:A:72:TYR:CD1	2.50	0.47
7:G:109:TYR:CE2	7:G:151:VAL:HG11	2.49	0.47
1:A:57:ASP:CG	6:F:156:ARG:HH12	2.18	0.47
2:B:161:ASP:HA	2:B:186:GLY:HA3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:ARG:HB3	5:E:117:TYR:CE2	2.50	0.47
1:A:351:GLU:C	1:A:353:LEU:H	2.18	0.47
3:C:116:GLY:C	3:C:118:ARG:N	2.67	0.47
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.96	0.47
4:D:277:LEU:CD1	6:F:102:PHE:HE1	2.28	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
4:D:267:ARG:HG3	4:D:267:ARG:NH1	2.30	0.47
4:D:75:LEU:C	4:D:75:LEU:HD23	2.35	0.47
3:C:144:THR:OG1	6:F:28:GLN:HG2	2.15	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:30:GLY:HA3	5:E:135:GLN:CD	2.35	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
1:A:327:MET:O	1:A:328:PHE:C	2.53	0.46
2:B:230:GLU:OE2	6:F:35:LYS:HE2	2.14	0.46
3:C:172:TYR:C	3:C:172:TYR:CD2	2.88	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
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
7:G:75:ALA:HA	7:G:78:ILE:HD12	1.96	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
3:C:265:CYS:SG	3:C:327:ASN:C	2.94	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:112:LEU:HD11	1:A:130:MET:HE2	1.96	0.46
1:A:228:LYS:O	1:A:232:SER:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TRP:CB	4:D:267:ARG:HE	2.29	0.46
3:C:21:THR:CG2	3:C:22:GLN:HG3	2.44	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
5:E:5:HIS:CD2	5:E:65:ASP:OD2	2.69	0.46
6:F:85:ILE:C	6:F:85:ILE:HD12	2.35	0.46
3:C:100:ARG:O	3:C:100:ARG:HG3	2.16	0.46
4:D:65:LYS:CE	4:D:65:LYS:H	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:HB3	1:A:230:ARG:HH11	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
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:183:ASP:C	2:B:184:ILE:HG13	2.35	0.45
2:B:259:PHE:CE2	2:B:260:GLU:HG3	2.51	0.45
3:C:354:MET:SD	3:C:354:MET:C	2.94	0.45
3:C:73:ASP:N	3:C:73:ASP:OD1	2.49	0.45
4:D:154:VAL:HG12	4:D:155:GLU:N	2.31	0.45
1:A:334:ARG:HG2	1:A:334:ARG:NH1	2.30	0.45
1:A:6:PRO:HG2	1:A:21:TYR:HD2	1.81	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
1:A:102:ARG:C	4:D:38:PHE:CE2	2.89	0.45
5:E:60:ILE:HD12	5:E:60:ILE:N	2.30	0.45
5:E:28:PHE:CD2	5:E:138:GLN:HB3	2.51	0.45
5:E:13:THR:HG21	5:E:22:LEU:CD1	2.47	0.45
7:G:68:SER:OG	7:G:71:VAL:HG12	2.16	0.45
1:A:111:LEU:CD2	1:A:111:LEU:C	2.84	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:343:SER:C	3:C:359:VAL:HG23	2.37	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:329:VAL:HG11	3:C:347:THR:HB	1.98	0.45
3:C:32:VAL:CG2	3:C:58:ILE:HD11	2.41	0.45
4:D:51:ASP:OD1	4:D:54:LYS:HD3	2.16	0.45
2:B:198:LEU:C	2:B:200:ARG:H	2.20	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
1:A:6:PRO:HG2	1:A:21:TYR:CD2	2.53	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
1:A:144:GLN:O	1:A:146:VAL:N	2.51	0.44
5:E:85:CYS:CB	5:E:90:GLN:HE22	2.30	0.44
2:B:236:GLU:O	6:F:105:ARG:HG2	2.17	0.44
3:C:265:CYS:SG	3:C:327:ASN:O	2.76	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:CA	2:B:231:GLN:HE21	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:101:LEU:O	1:A:102:ARG:C	2.56	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ILE:HG13	2:B:263:GLU:OE1	2.18	0.44
4:D:109:ILE:HG13	4:D:110:VAL:N	2.32	0.44
4:D:87:PRO:HB3	4:D:92:ASN:O	2.18	0.44
4:D:5:GLU:CD	4:D:9:ARG:HE	2.19	0.44
7:G:100:LYS:HA	7:G:100:LYS:HD3	1.72	0.44
2:B:190:THR:O	2:B:193:LEU:HB3	2.17	0.44
2:B:232:LYS:HB3	2:B:232:LYS:NZ	2.33	0.44
2:B:322:LYS:HD2	7:G:16:VAL:HG11	1.99	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
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:221:LEU:O	1:A:224:ALA:HB3	2.18	0.43
1:A:53:LYS:O	1:A:56:ASP:OD2	2.36	0.43
3:C:216:ARG:NH2	3:C:274:SER:HB2	2.33	0.43
3:C:69:THR:O	3:C:76:ALA:HA	2.18	0.43
4:D:147:ARG:O	4:D:148:ASP:C	2.55	0.43
4:D:53:THR:C	4:D:54:LYS:HD2	2.38	0.43
5:E:121:ALA:O	5:E:122:ASN:CB	2.61	0.43
6:F:104:LEU:HD23	6:F:104:LEU:HA	1.75	0.43
6:F:95:MET:HE2	6:F:108:PRO:HG3	1.99	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:77:LYS:C	6:F:78:GLN:HG3	2.38	0.43
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.53	0.43
4:D:228:PHE:O	4:D:229:PRO:C	2.57	0.43
4:D:84:LEU:HD23	4:D:85:VAL:H	1.84	0.43
6:F:60:LYS:HE3	6:F:112:TYR:CZ	2.53	0.43
1:A:151:ALA:O	1:A:154:THR:HG22	2.18	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
3:C:366:LEU:HB2	3:C:369:LEU:HB2	2.01	0.43
1:A:126:THR:OG1	8:A:501:C69:CAR	2.56	0.43
1:A:77:PRO:O	8:A:501:C69:H5	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PHE:HZ	1:A:277:LEU:HD11	1.82	0.43
3:C:13:CYS:HA	3:C:331:GLN:HE22	1.82	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:280:GLU:HG3	1:A:280:GLU:O	2.19	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:85:CYS:HB2	5:E:90:GLN:CD	2.38	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
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
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
6:F:101:PHE:O	6:F:104:LEU:HB2	2.19	0.42
7:G:27:GLU:HA	7:G:27:GLU:OE2	2.19	0.42
7:G:8:SER:C	7:G:10:ARG:N	2.72	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:HH11	2:B:180:ARG:HG3	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
4:D:199:LEU:HD12	4:D:199:LEU:N	2.34	0.42
5:E:150:ASP:O	5:E:152:GLN:N	2.52	0.42
5:E:85:CYS:CB	5:E:90:GLN:NE2	2.82	0.42
6:F:40:VAL:HG23	6:F:41:ARG:N	2.35	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
3:C:126:GLU:C	3:C:128:GLU:H	2.22	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
4:D:247:PHE:O	4:D:248:ARG:C	2.58	0.42
5:E:96:TYR:O	5:E:100:ILE:HG12	2.20	0.42
1:A:295:PRO:O	1:A:298:GLU:N	2.49	0.42
2:B:170:TYR:O	2:B:172:GLY:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:150:ASP:C	5:E:152:GLN:N	2.71	0.42
5:E:91:GLY:C	5:E:93:LYS:N	2.73	0.42
6:F:130:LYS:O	6:F:133:ASP:N	2.50	0.42
1:A:311:VAL:HG13	1:A:311:VAL:O	2.20	0.42
1:A:4:ARG:HD2	4:D:62:LYS:HE2	2.00	0.42
2:B:316:ARG:HG2	2:B:316:ARG:HH11	1.84	0.42
2:B:279:ALA:HB3	2:B:320:GLU:HG2	1.97	0.42
3:C:173:ILE:HD11	3:C:191:PHE:CE1	2.54	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
2:B:322:LYS:HD2	7:G:16:VAL:CG1	2.50	0.42
7:G:36:GLY:CA	7:G:63:PRO:HG3	2.48	0.42
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
7:G:79:VAL:HG11	7:G:109:TYR:HD1	1.83	0.42
1:A:80:HIS:CE1	1:A:192:HIS:CE1	3.06	0.42
1:A:79:ARG:HH11	1:A:79:ARG:CG	2.31	0.42
4:D:80:TYR:CD2	4:D:95:LEU:HD22	2.54	0.42
5:E:14:LYS:CA	5:E:14:LYS:HE2	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
6:F:8:TYR:CE2	6:F:139:MET:HE1	2.55	0.42
4:D:229:PRO:C	4:D:231:HIS:H	2.23	0.41
4:D:261:TYR:HE2	6:F:152:SER:OG	2.01	0.41
5:E:145:CYS:C	5:E:147:LYS:N	2.72	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:211:ARG:NH2	1:A:274:GLU:OE2	2.48	0.41
1:A:38:LYS:HG3	1:A:72:TYR:CD2	2.54	0.41
4:D:59:ILE:HG12	4:D:60:SER:N	2.34	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
6:F:139:MET:HB3	6:F:139:MET:HE2	1.93	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
1:A:64:ASP:C	1:A:66:ALA:N	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG	2:B:326:LEU:O	2.20	0.41
4:D:184:GLU:OE1	6:F:158:ARG:CB	2.67	0.41
4:D:75:LEU:O	4:D:75:LEU:HD23	2.20	0.41
5:E:16:ILE:CG1	5:E:129:MET:HB2	2.51	0.41
5:E:131:ALA:C	5:E:133:LEU:H	2.23	0.41
1:A:385:ALA:HA	1:A:390:PHE:CG	2.55	0.41
4:D:116:LEU:HD23	4:D:116:LEU:C	2.41	0.41
1:A:14:THR:HG22	1:A:15:GLY:N	2.34	0.41
2:B:326:LEU:C	2:B:326:LEU:HD23	2.41	0.41
3:C:112:ALA:HB1	3:C:148:LEU:HD13	2.03	0.41
3:C:6:PHE:CE2	3:C:35:TYR:CG	3.08	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:108:PRO:HB3	6:F:112:TYR:O	2.20	0.41
6:F:76:VAL:N	6:F:113:ASP:OD2	2.54	0.41
1:A:144:GLN:O	1:A:145:ALA:C	2.59	0.41
3:C:155:VAL:HG21	3:C:180:PRO:HG3	2.03	0.41
3:C:326:LYS:HA	3:C:326:LYS:HD3	1.78	0.41
5:E:76:SER:O	5:E:80:LYS:HG3	2.20	0.41
3:C:185:TRP:CZ2	3:C:231:ALA:HB2	2.56	0.41
4:D:184:GLU:OE1	6:F:158:ARG:NE	2.41	0.41
4:D:188:GLY:C	4:D:190:ARG:H	2.25	0.41
5:E:100:ILE:HA	5:E:134:GLN:NE2	2.27	0.41
5:E:58:TYR:CD2	5:E:69:ILE:HD11	2.55	0.41
6:F:52:THR:O	7:G:114:PHE:CD1	2.74	0.41
6:F:8:TYR:HE2	6:F:139:MET:CE	2.33	0.41
7:G:114:PHE:HA	7:G:114:PHE:HD2	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:CD2	1:A:202:TYR:N	2.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	3:C:118:ARG:HG3	2.34	0.40
4:D:176:VAL:HG21	6:F:85:ILE:HG21	2.03	0.40
1:A:211:ARG:HH11	5:E:159:TRP:HZ3	1.67	0.40
7:G:99:ASP:OD2	7:G:101:ASN:HB2	2.21	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
1:A:120:PRO:CG	2:B:201:GLY:HA3	2.51	0.40
2:B:255:GLY:O	2:B:256:GLY:C	2.60	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
1:A:258:GLY:C	1:A:259:ILE:HD12	2.40	0.40
4:D:277:LEU:HD12	6:F:102:PHE:HE1	1.86	0.40
4:D:64:TYR:CB	4:D:92:ASN:HD22	2.29	0.40
6:F:105:ARG:HG2	6:F:105:ARG:NH1	2.36	0.40
3:C:160:GLY:HA3	3:C:205:VAL:HG12	2.03	0.40
3:C:14:HIS:O	3:C:331:GLN:OE1	2.39	0.40
4:D:281:ARG:NH1	6:F:126:MET:CE	2.84	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
3:C:56:THR:OG1	3:C:70:CYS:O	2.38	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
3:C:144:THR:H	6:F:28:GLN:NE2	2.19	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	393/418 (94%)	317 (81%)	61 (16%)	15 (4%)	3 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	193/394 (49%)	150 (78%)	36 (19%)	7 (4%)	3 5
3	C	337/372 (91%)	302 (90%)	31 (9%)	4 (1%)	13 23
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%)	13 23
7	G	132/151 (87%)	109 (83%)	21 (16%)	2 (2%)	10 18
All	All	1663/1981 (84%)	1384 (83%)	230 (14%)	49 (3%)	4 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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/363 (96%)	332 (95%)	17 (5%)	25	43
2	B	163/345 (47%)	150 (92%)	13 (8%)	12	21
3	C	286/313 (91%)	272 (95%)	14 (5%)	25	43
4	D	239/264 (90%)	227 (95%)	12 (5%)	24	42
5	E	154/159 (97%)	148 (96%)	6 (4%)	32	52
6	F	153/155 (99%)	145 (95%)	8 (5%)	23	39
7	G	88/123 (72%)	83 (94%)	5 (6%)	20	36
All	All	1432/1722 (83%)	1357 (95%)	75 (5%)	23	39

All (75) 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	191	LYS
1	A	217	PRO
1	A	230	ARG
1	A	235	CYS
1	A	255	GLN
1	A	257	THR
1	A	282	PHE
1	A	289	ASN
1	A	335	LEU
1	A	363	ILE
1	A	406	SER
2	B	161	ASP
2	B	175	LEU
2	B	182	LEU
2	B	200	ARG
2	B	252	ILE
2	B	274	GLU
2	B	276	VAL
2	B	303	LEU
2	B	311	PRO
2	B	320	GLU
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	187	SER
3	C	210	PHE
3	C	321	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	140	ASN
4	D	141	ARG
4	D	160	ARG
4	D	171	ASP
4	D	204	GLU
4	D	229	PRO
4	D	258	SER
4	D	270	THR
5	E	22	LEU
5	E	38	ASP
5	E	67	THR
5	E	82	LEU
5	E	95	MET
5	E	144	LEU
6	F	6	ARG
6	F	22	LEU
6	F	66	SER
6	F	101	PHE
6	F	102	PHE
6	F	104	LEU
6	F	152	SER
6	F	165	LEU
7	G	15	ASP
7	G	29	ASP
7	G	90	ASP
7	G	104	ASP
7	G	114	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	205	GLN
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	395	HIS
2	B	205	ASN
2	B	231	GLN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	4	HIS
3	C	33	HIS
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	140	ASN
4	D	197	GLN
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
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	78	GLN
7	G	50	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 (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1.83	2 (8%)	33,35,35	2.51	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	501	C69	CAE-NAF	-7.65	1.33	1.43
8	A	501	C69	CAQ-NAF	-3.27	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	501	C69	CAQ-CAR-SAS	-7.79	100.94	107.60
8	A	501	C69	CAR-CAQ-NAF	7.10	116.99	112.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	501	C69	CAB-OAA-CAD	-5.17	109.73	117.53
8	A	501	C69	CAL-OAM-CAN	-4.31	108.15	117.51
8	A	501	C69	OAW-CAQ-NAF	-3.43	122.36	125.10
8	A	501	C69	OAA-CAD-CAC	-3.09	118.80	124.12
8	A	501	C69	OAA-CAD-CAE	2.93	120.05	116.06
8	A	501	C69	CAH-CAG-NAF	-2.02	111.29	113.49

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-CAQ
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

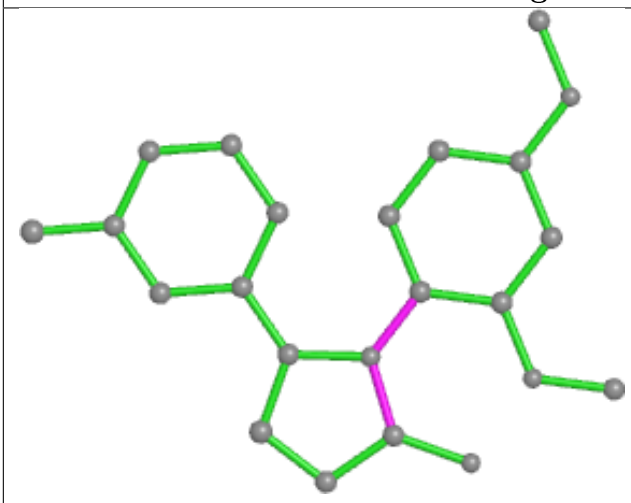
There are no ring outliers.

1 monomer is involved in 11 short contacts:

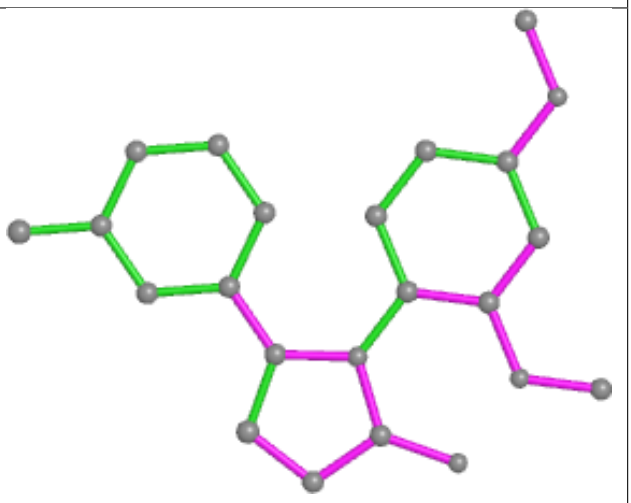
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	501	C69	11	0

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 then 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.

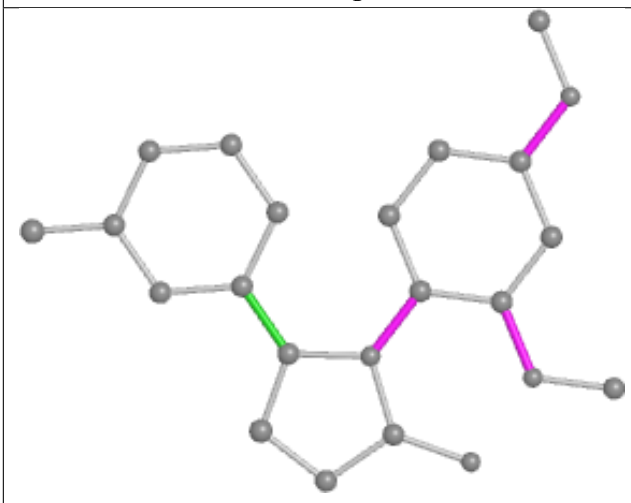
Ligand C69 A 501



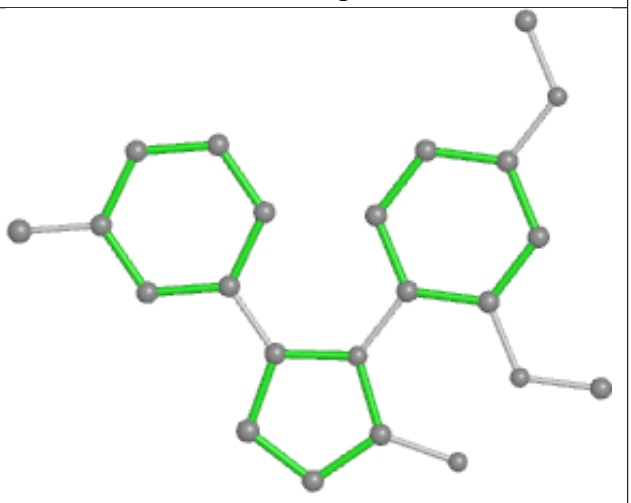
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	399/418 (95%)	0.19	14 (3%) 44 52	28, 60, 92, 107	0
2	B	195/394 (49%)	0.62	25 (12%) 3 4	35, 73, 109, 115	0
3	C	341/372 (91%)	0.01	0 100 100	32, 52, 78, 95	0
4	D	277/300 (92%)	0.08	4 (1%) 75 82	30, 60, 96, 114	0
5	E	173/178 (97%)	0.29	8 (4%) 32 39	52, 79, 111, 119	0
6	F	166/168 (98%)	-0.03	1 (0%) 89 92	28, 56, 74, 87	0
7	G	138/151 (91%)	0.50	11 (7%) 12 15	49, 100, 118, 120	0
All	All	1689/1981 (85%)	0.20	63 (3%) 41 49	28, 63, 105, 120	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	178	LEU	5.3
1	A	156	ARG	5.3
5	E	154	ASP	4.6
7	G	151	VAL	4.6
2	B	174	SER	4.4
1	A	161	ARG	4.2
7	G	49	GLY	4.1
1	A	360	PRO	4.1
5	E	153	ASN	4.1
5	E	85	CYS	4.0
2	B	181	ARG	4.0
7	G	50	ASN	3.8
5	E	89	SER	3.6
2	B	180	ARG	3.6
7	G	19	TYR	3.5
1	A	416	VAL	3.5
1	A	81	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	215	ALA	3.4
1	A	82	ILE	3.4
5	E	151	PRO	3.4
2	B	292	ASP	3.3
2	B	177	HIS	3.3
7	G	84	ILE	3.2
2	B	183	ASP	3.2
2	B	172	GLY	3.1
2	B	347	PRO	3.1
2	B	173	PHE	3.1
1	A	359	LYS	3.0
2	B	166	ILE	2.9
2	B	154	GLY	2.8
6	F	58	LYS	2.8
7	G	45	CYS	2.8
7	G	63	PRO	2.8
2	B	175	LEU	2.8
2	B	168	PRO	2.8
2	B	325	TYR	2.8
4	D	228	PHE	2.7
2	B	187	ARG	2.7
1	A	52	MET	2.6
2	B	170	TYR	2.5
1	A	157	GLN	2.5
1	A	97	ILE	2.4
2	B	293	THR	2.4
5	E	88	LYS	2.4
1	A	351	GLU	2.3
1	A	350	SER	2.3
2	B	329	VAL	2.3
7	G	48	GLN	2.3
4	D	216	VAL	2.3
7	G	46	LEU	2.2
2	B	340	PHE	2.2
2	B	155	VAL	2.2
1	A	354	SER	2.2
5	E	84	LYS	2.2
7	G	58	ALA	2.2
2	B	163	VAL	2.1
5	E	92	GLU	2.1
4	D	159	ASP	2.1
2	B	171	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	53	LYS	2.1
2	B	169	VAL	2.1
2	B	164	THR	2.0
7	G	55	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

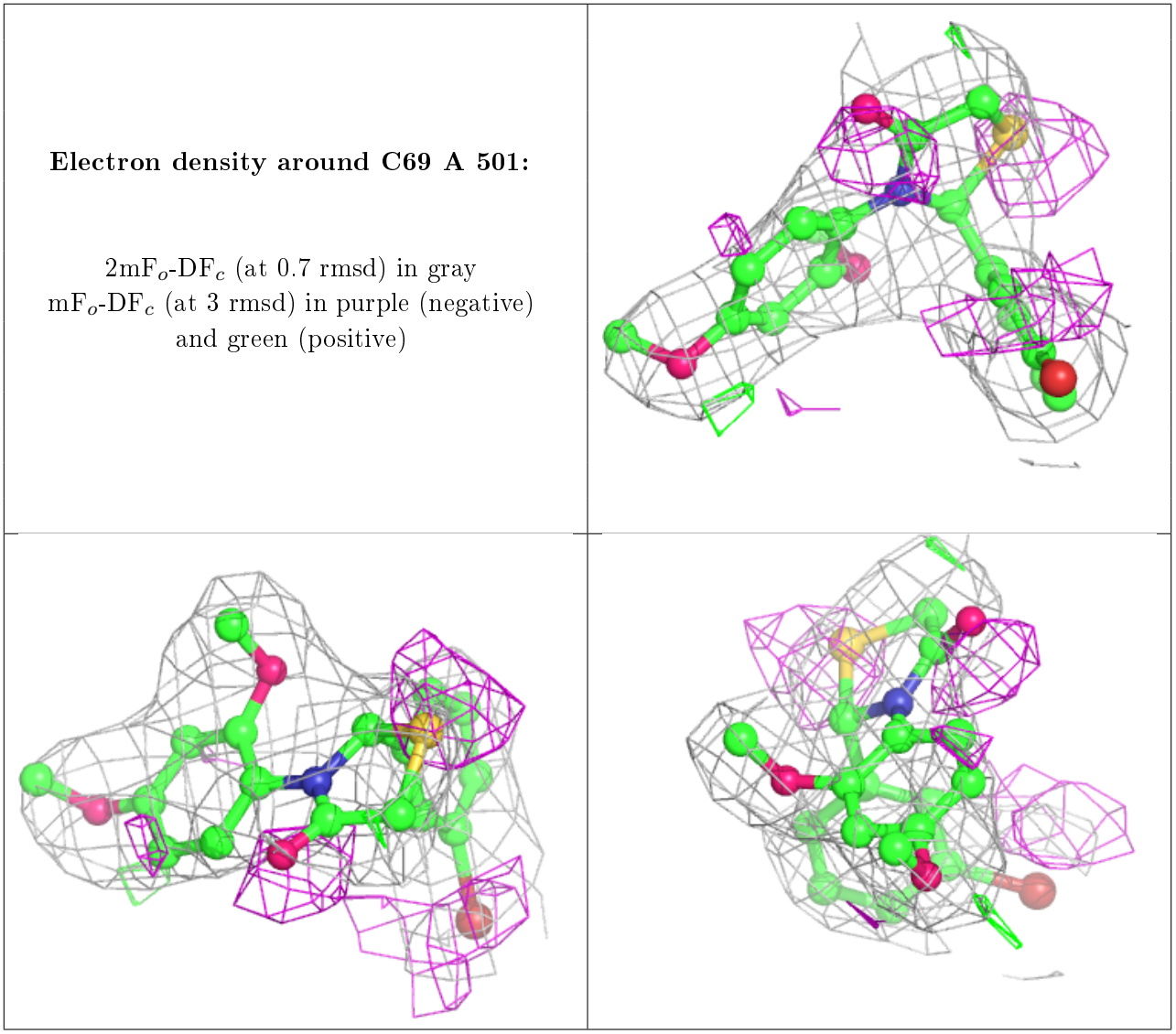
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	C69	A	501	23/23	0.92	0.24	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

There are no such residues in this entry.