



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:02 AM UTC

PDB ID : 3DXM / pdb_00003dxm
Title : Structure of Bos taurus Arp2/3 Complex with Bound Inhibitor CK0993548
Authors : Nolen, B.J.; Tomasevic, N.; Russell, A.; Pierce, D.W.; Jia, Z.; Hartman, J.; Sakowicz, R.; Pollard, T.D.
Deposited on : 2008-07-24
Resolution : 2.85 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

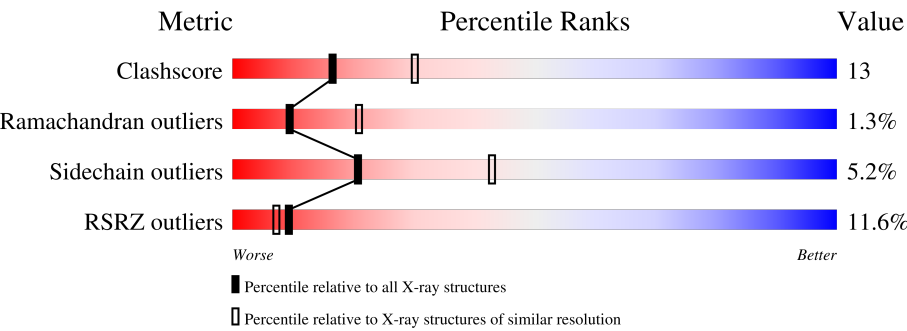
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	8% 70% 21% • 5%
2	B	394	15% 30% 14% 5% • 50%
3	C	372	3% 67% 22% • 8%
4	D	300	5% 80% 13% 6%
5	E	178	13% 62% 28% 7% • •
6	F	168	5% 83% 14% • • •
7	G	151	28% 67% 21% • 9%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13527 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-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3199	2055	534	595	15			

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1525	980	258	283	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
			2649	1681	464	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	281	Total	C	N	O	S	0	0	0
			2271	1445	394	424	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1400	897	235	259	9			

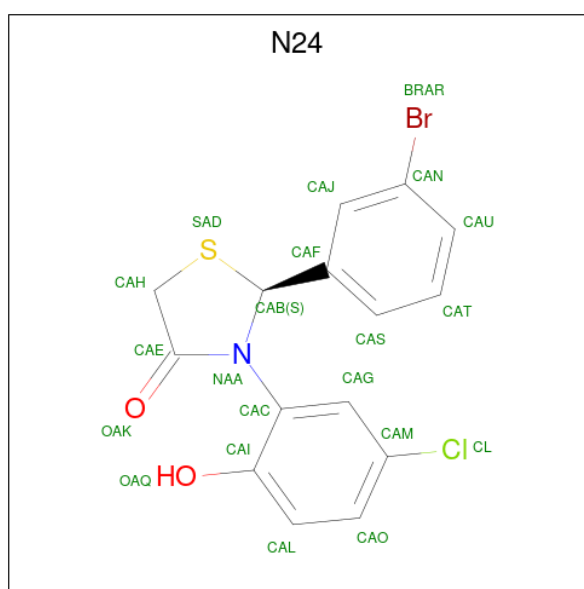
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	137	Total	C	N	O	S	0	0	0
			1044	652	183	206	3			

- Molecule 8 is (2S)-2-(3-bromophenyl)-3-(5-chloro-2-hydroxyphenyl)-1,3-thiazolidin-4-one (CCD ID: N24) (formula: C₁₅H₁₁BrClNO₂S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	A	1	Total	Br	C	Cl	N	O	S	0	0
			21	1	15	1	1	2	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	11	Total	O	0	0
			11	11		
9	B	2	Total	O	0	0
			2	2		
9	C	14	Total	O	0	0
			14	14		
9	D	9	Total	O	0	0
			9	9		

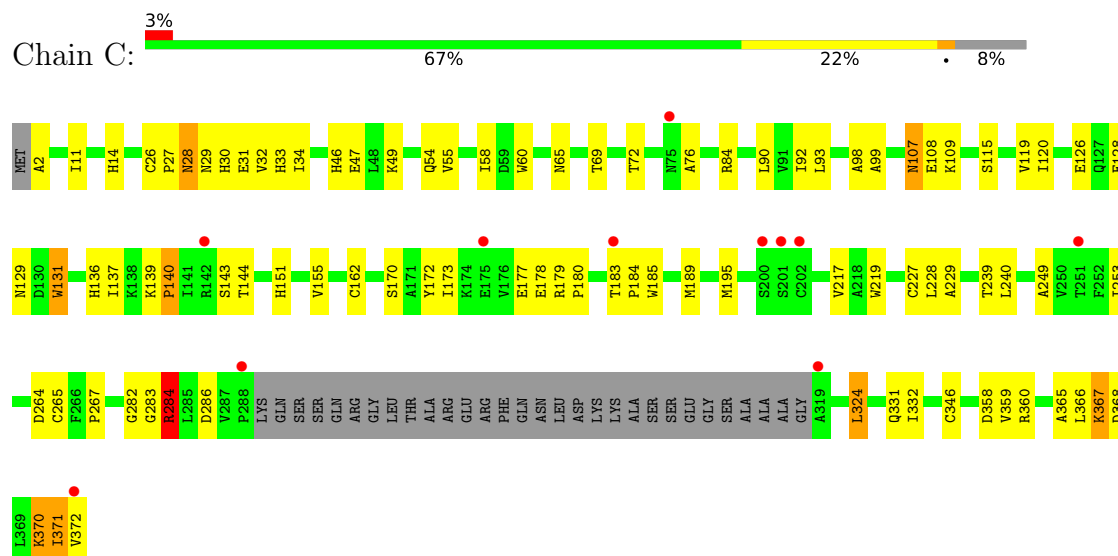
Continued on next page...

Continued from previous page...

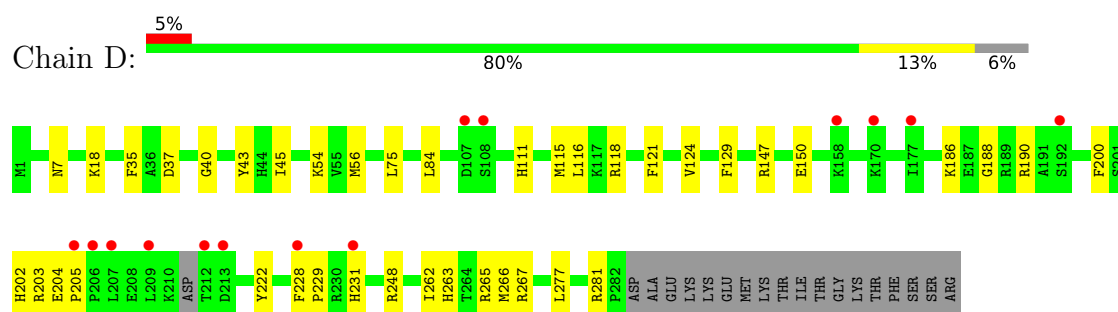
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	10	Total	O	0	0
			10	10		
9	G	1	Total	O	0	0
			1	1		

LEU
ALA
ASP
ILE
MET
LYS
LYS
ASP
ASN
PHE
TRP
MET
THR
ARG
GLN
GLU
TVR
GLN
GLY
VAL
ARG
VAL
LEU
GLU
LYS
LYS
GLY
GLY
VAL
THR
VAL
ARG

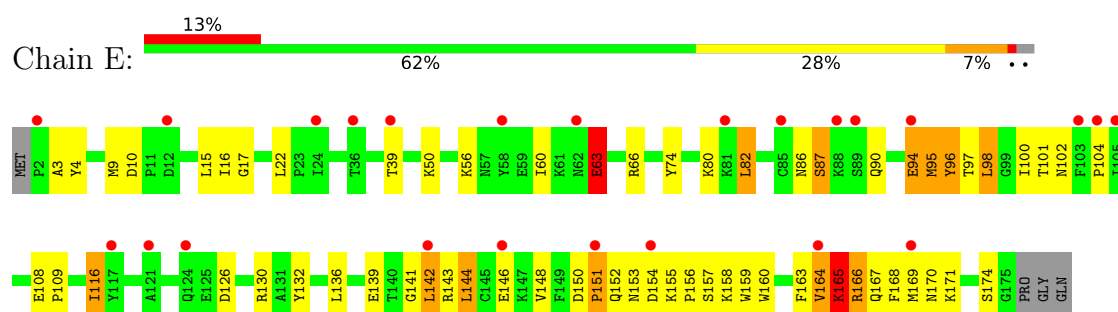
• Molecule 3: Actin-related protein 2/3 complex subunit 1B



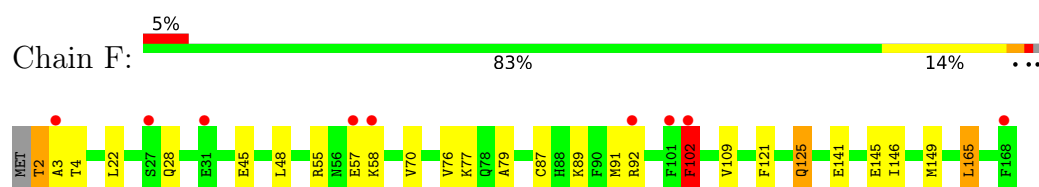
• Molecule 4: Actin-related protein 2/3 complex subunit 2



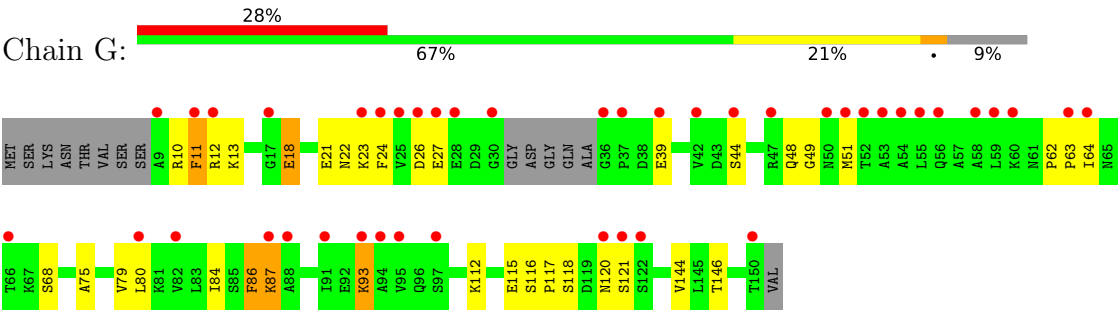
• Molecule 5: Actin-related protein 2/3 complex subunit 3



• 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	111.38Å 129.65Å 203.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.85) 91.8 (30.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.81Å)	Xtriage
Refinement program	CNS, REFMAC 5.0	Depositor
R, R_{free}	0.245 , 0.258 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13527	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: N24

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	0.39	0/3280	1.02	20/4450 (0.4%)
2	B	0.43	1/1555 (0.1%)	0.96	8/2110 (0.4%)
3	C	0.31	0/2718	0.95	11/3689 (0.3%)
4	D	0.30	0/2319	0.84	1/3129 (0.0%)
5	E	0.31	0/1433	0.98	8/1934 (0.4%)
6	F	0.33	0/1393	0.91	4/1868 (0.2%)
7	G	0.33	0/1056	0.90	2/1420 (0.1%)
All	All	0.35	1/13754 (0.0%)	0.95	54/18600 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	VAL	CA-CB	5.38	1.60	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	283	GLY	N-CA-C	11.34	126.57	111.72
5	E	166	ARG	N-CA-C	-10.53	94.10	110.42
1	A	78	ILE	CB-CA-C	-9.84	100.17	111.09
2	B	347	PRO	N-CA-C	9.35	122.11	110.70
5	E	165	LYS	N-CA-C	9.34	124.22	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	HIS	N-CA-C	-9.08	94.53	108.96
2	B	347	PRO	CA-C-N	9.08	130.53	120.45
2	B	347	PRO	C-N-CA	9.08	130.53	120.45
3	C	30	HIS	N-CA-C	-8.77	102.12	113.17
1	A	83	VAL	N-CA-C	8.54	127.11	109.34
3	C	11	ILE	N-CA-C	-8.47	94.89	107.51
1	A	83	VAL	CA-C-N	8.33	132.96	121.05
1	A	83	VAL	C-N-CA	8.33	132.96	121.05
2	B	301	ILE	N-CA-C	-8.21	96.62	108.36
7	G	144	VAL	N-CA-C	-8.17	102.92	111.58
1	A	78	ILE	N-CA-C	8.12	121.07	106.61
1	A	118	ASN	N-CA-C	-7.99	99.23	110.50
3	C	284	ARG	N-CA-C	-7.24	98.77	110.20
1	A	79	ARG	N-CA-C	7.14	119.71	108.79
1	A	85	ASP	N-CA-C	-6.73	96.69	108.20
5	E	174	SER	N-CA-C	-6.65	105.04	113.02
6	F	102	PHE	N-CA-C	6.61	124.89	110.80
1	A	373	GLN	N-CA-C	6.60	118.13	111.07
3	C	137	ILE	N-CA-C	-6.50	97.76	107.37
2	B	337	LEU	N-CA-C	-6.46	103.75	111.69
1	A	109	TYR	N-CA-C	-6.33	101.11	110.48
1	A	69	LYS	CA-C-N	6.30	127.72	119.84
1	A	69	LYS	C-N-CA	6.30	127.72	119.84
5	E	63	GLU	N-CA-C	-6.22	105.55	113.01
5	E	17	GLY	N-CA-C	-6.17	100.46	110.95
2	B	220	LEU	N-CA-C	5.99	120.72	113.41
4	D	129	PHE	N-CA-C	-5.89	104.94	111.36
2	B	177	HIS	N-CA-C	-5.87	101.16	109.96
6	F	109	VAL	N-CA-C	-5.80	102.09	109.58
5	E	109	PRO	N-CA-C	-5.79	101.41	111.32
3	C	28	ASN	N-CA-C	-5.77	103.69	111.54
1	A	284	HIS	CA-C-N	5.76	125.89	119.32
1	A	284	HIS	C-N-CA	5.76	125.89	119.32
1	A	68	GLU	N-CA-C	5.72	119.84	112.41
1	A	178	ILE	N-CA-C	5.61	116.58	107.71
3	C	151	HIS	N-CA-C	-5.53	102.66	110.29
3	C	115	SER	N-CA-C	5.52	116.65	108.86
6	F	79	ALA	N-CA-C	5.40	117.17	111.28
5	E	160	TRP	N-CA-C	-5.35	107.40	114.04
3	C	253	ILE	N-CA-C	-5.32	108.09	113.47
3	C	359	VAL	N-CA-C	5.28	116.01	110.62
6	F	141	GLU	N-CA-C	5.27	117.93	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LEU	N-CA-C	5.26	116.70	111.07
1	A	235	CYS	CA-C-N	5.24	124.74	119.19
1	A	235	CYS	C-N-CA	5.24	124.74	119.19
2	B	348	PRO	N-CA-C	5.17	120.81	114.35
3	C	99	ALA	N-CA-C	-5.07	102.97	110.48
5	E	96	TYR	N-CA-C	-5.05	105.69	111.14
7	G	112	LYS	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	172	GLY	Peptide

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	3199	0	3149	91	0
2	B	1525	0	1513	76	0
3	C	2649	0	2604	69	0
4	D	2271	0	2243	30	0
5	E	1400	0	1394	46	0
6	F	1371	0	1410	27	0
7	G	1044	0	1052	25	0
8	A	21	0	10	3	0
9	A	11	0	0	0	0
9	B	2	0	0	0	0
9	C	14	0	0	1	0
9	D	9	0	0	0	0
9	F	10	0	0	0	0
9	G	1	0	0	0	0
All	All	13527	0	13375	346	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 13.

All (346) 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)
4:D:7:ASN:OD1	4:D:115:MET:HG2	1.62	0.98
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.46	0.96
3:C:367:LYS:HD3	3:C:368:ASP:N	1.85	0.92
1:A:84:GLU:HB2	8:A:419:N24:CL	2.08	0.91
7:G:87:LYS:H	7:G:87:LYS:HD3	1.39	0.86
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.58	0.84
3:C:189:MET:HA	3:C:195:MET:HE1	1.60	0.84
1:A:116:PRO:O	1:A:117:LEU:HB2	1.76	0.84
2:B:344:ILE:HG22	2:B:346:ASP:OD1	1.75	0.84
3:C:14:HIS:H	3:C:331:GLN:HE22	1.24	0.84
6:F:4:THR:HG23	6:F:55:ARG:HE	1.42	0.82
2:B:156:VAL:HG13	2:B:302:VAL:HG13	1.64	0.79
2:B:169:VAL:HG13	2:B:173:PHE:C	2.08	0.79
2:B:302:VAL:HA	2:B:345:GLU:O	1.83	0.79
2:B:177:HIS:O	2:B:178:LEU:HB2	1.82	0.79
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.66	0.78
3:C:32:VAL:HG22	3:C:58:ILE:HD11	1.64	0.78
1:A:4:ARG:CB	1:A:4:ARG:HH11	1.98	0.77
1:A:13:GLY:O	1:A:78:ILE:HG21	1.84	0.77
1:A:55:VAL:HG12	1:A:55:VAL:O	1.84	0.77
3:C:358:ASP:OD1	3:C:360:ARG:HG2	1.86	0.76
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.68	0.75
2:B:165:HIS:CD2	2:B:181:ARG:HG2	2.22	0.74
2:B:165:HIS:HD2	2:B:181:ARG:HG2	1.53	0.74
2:B:205:ASN:HD22	2:B:208:ALA:H	1.36	0.73
2:B:303:LEU:HD23	2:B:303:LEU:N	2.04	0.72
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.70	0.72
2:B:323:GLN:HB3	7:G:11:PHE:O	1.90	0.71
1:A:84:GLU:CB	8:A:419:N24:CL	2.77	0.70
7:G:93:LYS:NZ	7:G:93:LYS:HB3	2.04	0.70
6:F:121:PHE:O	6:F:125:GLN:HG2	1.92	0.69
3:C:107:ASN:C	3:C:107:ASN:HD22	2.01	0.69
7:G:87:LYS:HD3	7:G:87:LYS:N	2.07	0.69
2:B:169:VAL:HG13	2:B:173:PHE:O	1.93	0.68
2:B:156:VAL:HG22	2:B:302:VAL:HG12	1.75	0.68
5:E:87:SER:HA	5:E:153:ASN:OD1	1.92	0.68
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.76	0.68
2:B:302:VAL:C	2:B:303:LEU:HD23	2.19	0.68
3:C:58:ILE:HG12	3:C:69:THR:HG22	1.75	0.68
6:F:2:THR:O	6:F:4:THR:N	2.27	0.67
1:A:78:ILE:O	1:A:79:ARG:HG2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.07	0.67
1:A:176:HIS:HD2	1:A:192:HIS:HD2	1.42	0.66
4:D:203:ARG:O	4:D:204:GLU:HG2	1.95	0.66
3:C:107:ASN:ND2	3:C:109:LYS:H	1.94	0.66
1:A:176:HIS:HD2	1:A:192:HIS:CD2	2.13	0.66
3:C:189:MET:HG2	3:C:195:MET:HE3	1.77	0.66
1:A:129:ILE:O	1:A:133:SER:HB2	1.96	0.66
1:A:84:GLU:HG3	1:A:86:TRP:NE1	2.11	0.65
5:E:126:ASP:OD2	5:E:130:ARG:NH1	2.29	0.65
3:C:368:ASP:O	3:C:370:LYS:NZ	2.30	0.65
1:A:55:VAL:O	1:A:55:VAL:CG1	2.45	0.65
3:C:72:THR:HA	3:C:98:ALA:HB1	1.79	0.65
5:E:86:ASN:O	5:E:87:SER:HB3	1.97	0.65
4:D:263:HIS:HD2	4:D:266:MET:CE	2.11	0.64
2:B:159:SER:HB2	2:B:164:THR:HG23	1.79	0.64
3:C:365:ALA:C	3:C:366:LEU:HD12	2.22	0.64
1:A:289:ASN:C	1:A:289:ASN:HD22	2.06	0.64
3:C:144:THR:H	6:F:28:GLN:NE2	1.95	0.64
4:D:228:PHE:H	4:D:231:HIS:HD2	1.45	0.64
1:A:78:ILE:O	1:A:78:ILE:HG22	1.96	0.63
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.28	0.63
4:D:37:ASP:HB2	4:D:43:TYR:HE1	1.64	0.63
5:E:150:ASP:OD1	5:E:151:PRO:HD2	1.99	0.63
2:B:320:GLU:HG3	7:G:11:PHE:HE1	1.63	0.62
5:E:90:GLN:HG2	5:E:94:GLU:OE2	1.98	0.62
1:A:190:ILE:C	1:A:191:LYS:HD3	2.25	0.62
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.81	0.62
1:A:289:ASN:ND2	1:A:291:ASP:H	1.97	0.62
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.34	0.62
6:F:146:ILE:HA	6:F:149:MET:CE	2.29	0.62
1:A:289:ASN:HD22	1:A:291:ASP:H	1.48	0.61
5:E:168:PHE:CE2	5:E:169:MET:HE2	2.36	0.61
5:E:150:ASP:C	5:E:152:GLN:H	2.08	0.61
3:C:107:ASN:HD22	3:C:108:GLU:N	1.97	0.60
7:G:10:ARG:O	7:G:12:ARG:N	2.34	0.60
2:B:168:PRO:HG2	2:B:178:LEU:O	2.01	0.60
6:F:2:THR:C	6:F:4:THR:H	2.09	0.60
6:F:2:THR:HG21	6:F:55:ARG:HH22	1.67	0.60
5:E:150:ASP:O	5:E:152:GLN:N	2.35	0.60
3:C:183:THR:HG22	3:C:185:TRP:H	1.65	0.60
2:B:214:ARG:NH1	2:B:218:GLU:OE2	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASP:OD1	5:E:50:LYS:HE3	2.01	0.60
2:B:170:TYR:O	2:B:171:GLU:C	2.45	0.59
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.38	0.59
1:A:230:ARG:HH11	1:A:230:ARG:CB	2.15	0.59
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.37	0.59
1:A:194:PRO:C	1:A:195:ILE:HD12	2.28	0.58
5:E:60:ILE:HD13	5:E:66:ARG:HG2	1.85	0.58
6:F:2:THR:CG2	6:F:55:ARG:HH22	2.17	0.58
2:B:286:ILE:HG21	2:B:298:TYR:CE2	2.39	0.58
1:A:310:ASP:OD1	1:A:310:ASP:N	2.19	0.58
2:B:155:VAL:O	2:B:301:ILE:HA	2.04	0.58
1:A:111:LEU:HD23	1:A:111:LEU:C	2.29	0.58
1:A:343:VAL:HG22	1:A:363:ILE:CD1	2.34	0.57
2:B:170:TYR:O	2:B:172:GLY:N	2.37	0.57
4:D:203:ARG:O	4:D:203:ARG:HG2	2.04	0.57
5:E:95:MET:HA	5:E:95:MET:CE	2.34	0.57
3:C:370:LYS:HE2	3:C:370:LYS:H	1.68	0.57
1:A:216:PRO:HB2	1:A:219:GLN:HB2	1.85	0.57
2:B:161:ASP:O	2:B:187:ARG:HG3	2.05	0.57
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.35	0.57
4:D:248:ARG:HD3	4:D:248:ARG:C	2.30	0.57
3:C:27:PRO:HG2	3:C:29:ASN:HB2	1.86	0.57
3:C:84:ARG:O	3:C:84:ARG:HG2	2.04	0.57
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.85	0.57
5:E:16:ILE:HG23	5:E:16:ILE:O	2.05	0.57
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.40	0.56
1:A:359:LYS:N	1:A:360:PRO:HD3	2.20	0.56
3:C:126:GLU:C	3:C:128:GLU:H	2.13	0.56
3:C:371:ILE:O	3:C:372:VAL:HB	2.05	0.56
1:A:84:GLU:HG3	1:A:86:TRP:HE1	1.69	0.56
5:E:95:MET:HA	5:E:95:MET:HE3	1.86	0.56
2:B:166:ILE:O	2:B:168:PRO:HD3	2.06	0.55
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.87	0.55
3:C:264:ASP:O	3:C:265:CYS:HB2	2.07	0.55
5:E:86:ASN:O	5:E:87:SER:CB	2.54	0.55
1:A:19:LEU:HG	1:A:29:PHE:HB2	1.89	0.55
2:B:160:GLY:O	2:B:185:ALA:HB1	2.06	0.55
3:C:131:TRP:HE3	3:C:131:TRP:O	1.90	0.55
2:B:347:PRO:HB2	2:B:348:PRO:HD2	1.88	0.55
1:A:309:ILE:HA	1:A:312:ARG:HG3	1.89	0.55
2:B:217:LYS:O	2:B:221:CYS:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:LYS:HA	2:B:343:ARG:O	2.07	0.55
2:B:323:GLN:CD	7:G:12:ARG:HA	2.32	0.54
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.38	0.54
1:A:82:ILE:C	1:A:82:ILE:HD12	2.33	0.54
3:C:228:LEU:C	3:C:228:LEU:HD23	2.33	0.54
1:A:359:LYS:O	1:A:359:LYS:HD3	2.08	0.54
3:C:170:SER:HB2	3:C:195:MET:CE	2.37	0.54
7:G:18:GLU:OE1	7:G:23:LYS:NZ	2.40	0.54
1:A:82:ILE:HD12	1:A:82:ILE:O	2.07	0.54
3:C:173:ILE:O	3:C:177:GLU:HG2	2.07	0.54
2:B:318:GLU:CG	2:B:344:ILE:HG13	2.37	0.54
5:E:139:GLU:O	5:E:142:LEU:HD23	2.07	0.54
2:B:326:LEU:HD23	2:B:326:LEU:C	2.33	0.53
7:G:24:PHE:HE2	7:G:26:ASP:OD1	1.91	0.53
1:A:4:ARG:HH11	1:A:4:ARG:HB2	1.70	0.53
1:A:262:ILE:O	1:A:263:SER:CB	2.56	0.53
4:D:121:PHE:O	4:D:124:VAL:HG12	2.08	0.53
5:E:150:ASP:C	5:E:152:GLN:N	2.63	0.53
3:C:172:TYR:OH	3:C:179:ARG:HD2	2.08	0.53
1:A:55:VAL:HG13	1:A:58:LEU:HD12	1.90	0.53
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.90	0.53
2:B:330:LEU:C	2:B:332:GLY:H	2.17	0.53
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.43	0.53
3:C:367:LYS:HD3	3:C:367:LYS:C	2.33	0.53
3:C:370:LYS:O	3:C:371:ILE:HB	2.09	0.53
6:F:145:GLU:O	6:F:149:MET:HG3	2.09	0.52
3:C:26:CYS:SG	3:C:55:VAL:HB	2.49	0.52
4:D:186:LYS:NZ	4:D:200:PHE:H	2.07	0.52
7:G:93:LYS:HB3	7:G:93:LYS:HZ2	1.75	0.52
2:B:340:PHE:CZ	2:B:342:ILE:HD11	2.45	0.52
6:F:146:ILE:HA	6:F:149:MET:HE2	1.90	0.52
2:B:169:VAL:HG22	2:B:174:SER:HA	1.91	0.52
5:E:144:LEU:HD22	5:E:148:VAL:HG23	1.91	0.52
1:A:132:GLU:OE1	6:F:92:ARG:NH2	2.30	0.52
2:B:163:VAL:HG22	2:B:164:THR:H	1.75	0.52
6:F:89:LYS:HA	6:F:92:ARG:NH1	2.25	0.52
5:E:132:TYR:CE2	5:E:136:LEU:HD11	2.45	0.51
1:A:361:LYS:HG2	1:A:362:PRO:HD2	1.92	0.51
3:C:32:VAL:CG2	3:C:58:ILE:HD11	2.35	0.51
3:C:144:THR:CB	6:F:28:GLN:HE21	2.23	0.51
6:F:87:CYS:O	6:F:91:MET:HG2	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:146:ILE:HA	6:F:149:MET:HE3	1.93	0.51
5:E:165:LYS:O	5:E:165:LYS:HG2	2.09	0.51
3:C:178:GLU:O	3:C:179:ARG:C	2.54	0.51
1:A:176:HIS:CD2	1:A:192:HIS:HD2	2.27	0.50
1:A:359:LYS:O	1:A:359:LYS:CG	2.58	0.50
4:D:265:ARG:HD3	6:F:145:GLU:OE2	2.11	0.50
5:E:155:LYS:O	5:E:157:SER:N	2.43	0.50
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.46	0.50
2:B:303:LEU:N	2:B:303:LEU:CD2	2.74	0.50
2:B:318:GLU:HG3	2:B:344:ILE:HG13	1.93	0.50
3:C:14:HIS:H	3:C:331:GLN:NE2	2.03	0.50
3:C:32:VAL:HG22	3:C:58:ILE:CD1	2.39	0.50
1:A:409:ARG:HD3	2:B:200:ARG:O	2.10	0.50
2:B:299:LYS:HB3	2:B:343:ARG:CB	2.42	0.50
3:C:119:VAL:HG22	3:C:120:ILE:N	2.26	0.50
3:C:183:THR:HG21	3:C:185:TRP:HD1	1.76	0.50
2:B:163:VAL:HG22	2:B:164:THR:N	2.26	0.49
4:D:45:ILE:HA	4:D:56:MET:O	2.12	0.49
1:A:371:HIS:CD2	1:A:372:MET:SD	3.05	0.49
1:A:370:HIS:HD2	1:A:372:MET:H	1.58	0.49
5:E:9:MET:SD	5:E:63:GLU:HG2	2.53	0.49
5:E:95:MET:HG2	5:E:141:GLY:C	2.38	0.49
7:G:116:SER:N	7:G:117:PRO:HD3	2.28	0.49
2:B:169:VAL:HG22	2:B:174:SER:CA	2.43	0.49
3:C:107:ASN:C	3:C:107:ASN:ND2	2.67	0.49
3:C:189:MET:HG2	3:C:195:MET:CE	2.42	0.49
2:B:173:PHE:CG	2:B:174:SER:N	2.79	0.49
1:A:71:THR:HG23	1:A:72:TYR:CE1	2.48	0.49
1:A:190:ILE:O	1:A:191:LYS:HD3	2.13	0.48
7:G:23:LYS:HG2	7:G:24:PHE:H	1.77	0.48
4:D:7:ASN:HD21	4:D:111:HIS:CE1	2.30	0.48
1:A:15:GLY:O	1:A:16:TYR:CG	2.66	0.48
3:C:31:GLU:OE1	3:C:33:HIS:HE1	1.97	0.48
3:C:143:SER:OG	3:C:162:CYS:HB2	2.14	0.48
4:D:188:GLY:HA3	6:F:165:LEU:HD23	1.95	0.48
2:B:347:PRO:CB	2:B:348:PRO:HD2	2.44	0.48
7:G:24:PHE:CE2	7:G:26:ASP:OD1	2.66	0.48
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.96	0.48
5:E:152:GLN:HB2	5:E:155:LYS:CD	2.31	0.48
5:E:165:LYS:O	5:E:165:LYS:CG	2.62	0.48
2:B:180:ARG:HB2	2:B:281:LEU:HD21	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:167:GLN:HB3	5:E:171:LYS:O	2.14	0.47
4:D:7:ASN:OD1	4:D:115:MET:CG	2.49	0.47
5:E:60:ILE:HD12	5:E:116:ILE:HG23	1.96	0.47
1:A:343:VAL:HG22	1:A:363:ILE:HD12	1.95	0.47
5:E:104:PRO:HA	5:E:108:GLU:OE1	2.14	0.47
1:A:5:LEU:HD11	4:D:40:GLY:HA2	1.96	0.47
1:A:308:PRO:O	1:A:311:VAL:HG12	2.15	0.47
2:B:170:TYR:CE1	2:B:293:THR:HG21	2.50	0.47
3:C:282:GLY:O	3:C:370:LYS:HE3	2.15	0.47
3:C:219:TRP:CE2	3:C:227:CYS:HB2	2.50	0.47
4:D:75:LEU:HD23	4:D:75:LEU:C	2.39	0.47
1:A:239:VAL:HG23	1:A:240:LYS:N	2.29	0.47
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.97	0.47
1:A:76:TRP:C	1:A:78:ILE:H	2.22	0.47
3:C:367:LYS:HD3	3:C:368:ASP:H	1.75	0.47
2:B:169:VAL:HA	2:B:174:SER:HA	1.97	0.46
2:B:177:HIS:O	2:B:178:LEU:CB	2.56	0.46
1:A:123:ARG:HH12	2:B:201:GLY:CA	2.29	0.46
2:B:170:TYR:N	2:B:173:PHE:O	2.38	0.46
3:C:14:HIS:N	3:C:331:GLN:HE22	2.04	0.46
5:E:97:THR:O	5:E:101:THR:HG23	2.15	0.46
1:A:311:VAL:C	1:A:314:PRO:HD2	2.40	0.46
3:C:217:VAL:HG12	3:C:229:ALA:HB3	1.96	0.46
1:A:239:VAL:HG13	5:E:4:TYR:CZ	2.50	0.46
6:F:22:LEU:HD21	6:F:70:VAL:HG23	1.98	0.46
2:B:314:PRO:O	2:B:344:ILE:HD12	2.16	0.46
6:F:89:LYS:HA	6:F:92:ARG:HH12	1.80	0.46
7:G:118:SER:O	7:G:121:SER:HB3	2.15	0.46
2:B:157:VAL:HG13	2:B:166:ILE:HG12	1.98	0.46
6:F:57:GLU:HG3	6:F:58:LYS:HG2	1.98	0.46
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.51	0.45
1:A:76:TRP:HB2	1:A:79:ARG:HH12	1.81	0.45
3:C:34:ILE:HB	3:C:46:HIS:HB2	1.97	0.45
2:B:165:HIS:NE2	2:B:181:ARG:NE	2.65	0.45
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.32	0.45
1:A:4:ARG:HH11	1:A:4:ARG:HG2	1.80	0.45
6:F:2:THR:CG2	6:F:55:ARG:NH2	2.80	0.45
7:G:49:GLY:HA2	7:G:51:MET:HE2	1.99	0.45
3:C:170:SER:HB2	3:C:195:MET:HE3	1.98	0.45
1:A:359:LYS:O	1:A:359:LYS:CD	2.65	0.45
2:B:344:ILE:CG2	2:B:346:ASP:OD1	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:50:LYS:NZ	5:E:159:TRP:O	2.49	0.45
1:A:217:PRO:C	1:A:219:GLN:H	2.25	0.45
1:A:343:VAL:HG22	1:A:363:ILE:HD11	1.98	0.45
1:A:230:ARG:HH11	1:A:230:ARG:HB3	1.81	0.45
4:D:203:ARG:C	4:D:204:GLU:HG2	2.42	0.45
3:C:119:VAL:HG21	3:C:136:HIS:HB3	1.99	0.44
1:A:135:ASN:HB3	1:A:397:LYS:NZ	2.31	0.44
4:D:35:PHE:N	4:D:35:PHE:CD2	2.85	0.44
6:F:4:THR:CG2	6:F:55:ARG:HE	2.23	0.44
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.99	0.44
7:G:51:MET:HB3	7:G:86:PHE:CE1	2.53	0.44
5:E:95:MET:HE3	5:E:95:MET:CA	2.48	0.44
3:C:179:ARG:HA	3:C:180:PRO:HD3	1.84	0.44
1:A:116:PRO:O	1:A:117:LEU:CB	2.54	0.44
1:A:248:ASP:OD1	1:A:251:LYS:NZ	2.45	0.44
1:A:18:LYS:N	1:A:18:LYS:HD3	2.33	0.43
3:C:239:THR:HG22	3:C:240:LEU:N	2.33	0.43
5:E:82:LEU:HD23	5:E:148:VAL:HG21	1.99	0.43
1:A:108:HIS:O	1:A:137:PRO:HD2	2.18	0.43
1:A:311:VAL:O	1:A:314:PRO:HD2	2.18	0.43
5:E:96:TYR:O	5:E:100:ILE:HG12	2.18	0.43
5:E:102:ASN:HD21	5:E:130:ARG:HE	1.65	0.43
7:G:10:ARG:HG2	7:G:13:LYS:HD2	2.00	0.43
2:B:337:LEU:O	2:B:338:SER:C	2.62	0.43
3:C:2:ALA:N	9:C:373:HOH:O	2.51	0.43
6:F:121:PHE:O	6:F:125:GLN:CG	2.65	0.43
5:E:163:PHE:O	5:E:165:LYS:N	2.51	0.43
1:A:237:ASP:OD2	1:A:239:VAL:HG22	2.17	0.43
2:B:278:VAL:HG13	2:B:279:ALA:N	2.32	0.43
7:G:93:LYS:HB3	7:G:93:LYS:HZ3	1.80	0.43
1:A:4:ARG:CG	1:A:4:ARG:NH1	2.75	0.43
7:G:75:ALA:O	7:G:79:VAL:HG23	2.18	0.43
1:A:4:ARG:HB2	1:A:4:ARG:NH1	2.33	0.43
1:A:191:LYS:HE2	1:A:303:VAL:CG2	2.40	0.43
5:E:156:PRO:O	5:E:157:SER:C	2.61	0.43
3:C:27:PRO:O	3:C:28:ASN:C	2.59	0.43
3:C:284:ARG:NH1	3:C:286:ASP:O	2.40	0.43
1:A:244:LYS:HD3	1:A:252:TRP:CZ2	2.54	0.43
2:B:164:THR:HB	2:B:182:LEU:CB	2.49	0.43
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.49	0.43
1:A:202:TYR:O	1:A:205:GLN:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:154:ASP:CG	5:E:154:ASP:O	2.59	0.42
1:A:312:ARG:O	1:A:315:LEU:N	2.51	0.42
1:A:313:ARG:HB2	1:A:314:PRO:HD3	2.00	0.42
1:A:369:THR:HA	1:A:373:GLN:OE1	2.19	0.42
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.78	0.42
3:C:69:THR:O	3:C:76:ALA:HA	2.20	0.42
4:D:262:ILE:O	4:D:266:MET:HG3	2.19	0.42
5:E:139:GLU:O	5:E:143:ARG:HB2	2.18	0.42
2:B:318:GLU:HG3	2:B:344:ILE:CD1	2.49	0.42
2:B:157:VAL:O	2:B:303:LEU:HA	2.19	0.42
2:B:175:LEU:HD23	2:B:175:LEU:N	2.34	0.42
3:C:126:GLU:C	3:C:128:GLU:N	2.78	0.42
3:C:332:ILE:HA	3:C:346:CYS:O	2.19	0.42
4:D:186:LYS:HZ1	4:D:200:PHE:H	1.68	0.42
2:B:175:LEU:CD1	2:B:178:LEU:HD12	2.49	0.42
2:B:337:LEU:HD23	2:B:340:PHE:HB3	2.02	0.42
3:C:47:GLU:HG2	3:C:49:LYS:HE3	2.02	0.42
4:D:118:ARG:HD3	4:D:118:ARG:C	2.45	0.42
4:D:228:PHE:H	4:D:231:HIS:CD2	2.32	0.42
1:A:126:THR:OG1	8:A:419:N24:HAHA	2.19	0.42
3:C:60:TRP:HE1	3:C:65:ASN:ND2	2.17	0.42
3:C:267:PRO:HD2	3:C:286:ASP:HB2	2.01	0.42
3:C:366:LEU:HD12	3:C:366:LEU:N	2.35	0.42
7:G:44:SER:O	7:G:48:GLN:HG3	2.19	0.42
1:A:309:ILE:HG23	1:A:310:ASP:N	2.35	0.41
3:C:76:ALA:HB2	3:C:93:LEU:HD11	2.02	0.41
2:B:333:ASP:O	2:B:334:VAL:C	2.64	0.41
2:B:156:VAL:HA	2:B:302:VAL:O	2.20	0.41
1:A:84:GLU:CD	1:A:84:GLU:H	2.29	0.41
1:A:285:PRO:HG2	1:A:294:GLN:O	2.21	0.41
7:G:80:LEU:O	7:G:84:ILE:HD13	2.21	0.41
4:D:202:HIS:O	4:D:203:ARG:HB3	2.20	0.41
1:A:151:ALA:O	1:A:154:THR:HG22	2.21	0.41
1:A:343:VAL:HG11	1:A:363:ILE:HG13	2.03	0.41
2:B:169:VAL:HG22	2:B:174:SER:CB	2.51	0.41
2:B:231:GLN:NE2	2:B:231:GLN:HA	2.36	0.41
3:C:324:LEU:HD12	3:C:324:LEU:HA	1.91	0.41
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.51	0.41
6:F:48:LEU:HD22	7:G:146:THR:HG22	2.03	0.41
1:A:270:ASP:OD2	5:E:158:LYS:NZ	2.52	0.41
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:281:ARG:NH1	6:F:102:PHE:CZ	2.89	0.41
2:B:164:THR:HB	2:B:182:LEU:HB3	2.03	0.40
4:D:228:PHE:HB3	4:D:229:PRO:HD2	2.03	0.40
5:E:74:TYR:OH	5:E:98:LEU:HD12	2.20	0.40
5:E:95:MET:HG2	5:E:141:GLY:CA	2.50	0.40
1:A:140:TYR:HB2	1:A:394:CYS:SG	2.62	0.40
2:B:254:VAL:HG13	2:B:257:GLU:CG	2.50	0.40
3:C:29:ASN:O	3:C:54:GLN:HA	2.20	0.40
3:C:139:LYS:HA	3:C:140:PRO:HA	1.80	0.40
7:G:115:GLU:C	7:G:117:PRO:HD3	2.46	0.40
1:A:82:ILE:C	1:A:82:ILE:CD1	2.93	0.40
1:A:329:ARG:O	1:A:330:ASP:HB2	2.21	0.40
6:F:76:VAL:HG12	6:F:77:LYS:N	2.37	0.40
2:B:340:PHE:C	2:B:340:PHE:CD1	2.97	0.40
4:D:263:HIS:O	4:D:267:ARG:HG3	2.22	0.40
5:E:164:VAL:O	5:E:164:VAL:HG22	2.20	0.40
1:A:176:HIS:CD2	1:A:192:HIS:CD2	3.03	0.40
1:A:361:LYS:HG2	1:A:362:PRO:CD	2.52	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%)	370 (94%)	18 (5%)	5 (1%)	9	21
2	B	194/394 (49%)	164 (84%)	22 (11%)	8 (4%)	2	4
3	C	337/372 (91%)	317 (94%)	19 (6%)	1 (0%)	36	54
4	D	277/300 (92%)	273 (99%)	4 (1%)	0	100	100
5	E	172/178 (97%)	161 (94%)	7 (4%)	4 (2%)	5	11
6	F	165/168 (98%)	159 (96%)	4 (2%)	2 (1%)	10	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	133/151 (88%)	126 (95%)	5 (4%)	2 (2%)	8	18
All	All	1671/1981 (84%)	1570 (94%)	79 (5%)	22 (1%)	9	21

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	171	GLU
2	B	336	LYS
2	B	347	PRO
5	E	87	SER
6	F	3	ALA
7	G	11	PHE
7	G	22	ASN
5	E	3	ALA
6	F	102	PHE
1	A	83	VAL
1	A	117	LEU
1	A	263	SER
2	B	178	LEU
2	B	289	ALA
2	B	307	SER
5	E	164	VAL
1	A	312	ARG
5	E	151	PRO
3	C	371	ILE
2	B	335	GLU
1	A	70	PRO
2	B	155	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/363 (96%)	334 (95%)	16 (5%)	24	48
2	B	161/345 (47%)	143 (89%)	18 (11%)	6	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	290/313 (93%)	281 (97%)	9 (3%)	35	60
4	D	247/264 (94%)	241 (98%)	6 (2%)	43	67
5	E	153/159 (96%)	138 (90%)	15 (10%)	7	16
6	F	154/155 (99%)	151 (98%)	3 (2%)	50	72
7	G	112/123 (91%)	102 (91%)	10 (9%)	9	20
All	All	1467/1722 (85%)	1390 (95%)	77 (5%)	21	43

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	19	LEU
1	A	71	THR
1	A	117	LEU
1	A	143	VAL
1	A	191	LYS
1	A	230	ARG
1	A	251	LYS
1	A	255	GLN
1	A	265	LYS
1	A	310	ASP
1	A	335	LEU
1	A	343	VAL
1	A	349	LEU
1	A	353	LEU
1	A	363	ILE
2	B	155	VAL
2	B	171	GLU
2	B	175	LEU
2	B	182	LEU
2	B	184	ILE
2	B	220	LEU
2	B	231	GLN
2	B	274	GLU
2	B	290	ASP
2	B	299	LYS
2	B	303	LEU
2	B	320	GLU
2	B	326	LEU
2	B	337	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	338	SER
2	B	342	ILE
2	B	344	ILE
2	B	346	ASP
3	C	90	LEU
3	C	92	ILE
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	284	ARG
3	C	324	LEU
3	C	367	LYS
3	C	370	LYS
4	D	18	LYS
4	D	54	LYS
4	D	84	LEU
4	D	116	LEU
4	D	190	ARG
4	D	277	LEU
5	E	10	ASP
5	E	22	LEU
5	E	39	THR
5	E	63	GLU
5	E	80	LYS
5	E	82	LEU
5	E	94	GLU
5	E	95	MET
5	E	98	LEU
5	E	116	ILE
5	E	142	LEU
5	E	144	LEU
5	E	146	GLU
5	E	165	LYS
5	E	166	ARG
6	F	2	THR
6	F	125	GLN
6	F	165	LEU
7	G	18	GLU
7	G	21	GLU
7	G	27	GLU
7	G	39	GLU
7	G	64	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	68	SER
7	G	86	PHE
7	G	87	LYS
7	G	93	LYS
7	G	120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	176	HIS
1	A	192	HIS
1	A	255	GLN
1	A	289	ASN
1	A	318	ASN
1	A	370	HIS
1	A	371	HIS
1	A	392	GLN
1	A	395	HIS
2	B	205	ASN
2	B	231	GLN
2	B	284	ASN
2	B	323	GLN
3	C	30	HIS
3	C	33	HIS
3	C	65	ASN
3	C	107	ASN
3	C	129	ASN
3	C	331	GLN
4	D	111	HIS
4	D	140	ASN
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
4	D	278	ASN
5	E	102	ASN
6	F	28	GLN
6	F	120	ASN
6	F	125	GLN
6	F	137	HIS
7	G	22	ASN
7	G	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	96	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	N24	A	419	-	23,23,23	1.77	3 (13%)	31,33,33	1.77	8 (25%)

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	N24	A	419	-	-	0/8/21/21	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	419	N24	CAC-NAA	-5.76	1.36	1.43
8	A	419	N24	CAB-SAD	-3.85	1.79	1.84
8	A	419	N24	CAM-CL	2.37	1.80	1.74

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	419	N24	CAH-CAE-NAA	5.03	115.52	112.14
8	A	419	N24	CAE-CAH-SAD	-3.99	104.17	107.61
8	A	419	N24	CAF-CAB-SAD	2.59	115.53	111.60
8	A	419	N24	CAH-SAD-CAB	2.48	96.90	93.16
8	A	419	N24	CAF-CAJ-CAN	2.48	121.40	119.50
8	A	419	N24	CAI-CAC-NAA	2.32	122.25	119.42
8	A	419	N24	OAK-CAE-CAH	-2.30	118.94	123.64
8	A	419	N24	CAO-CAM-CAG	-2.19	118.67	121.53

There are no chirality outliers.

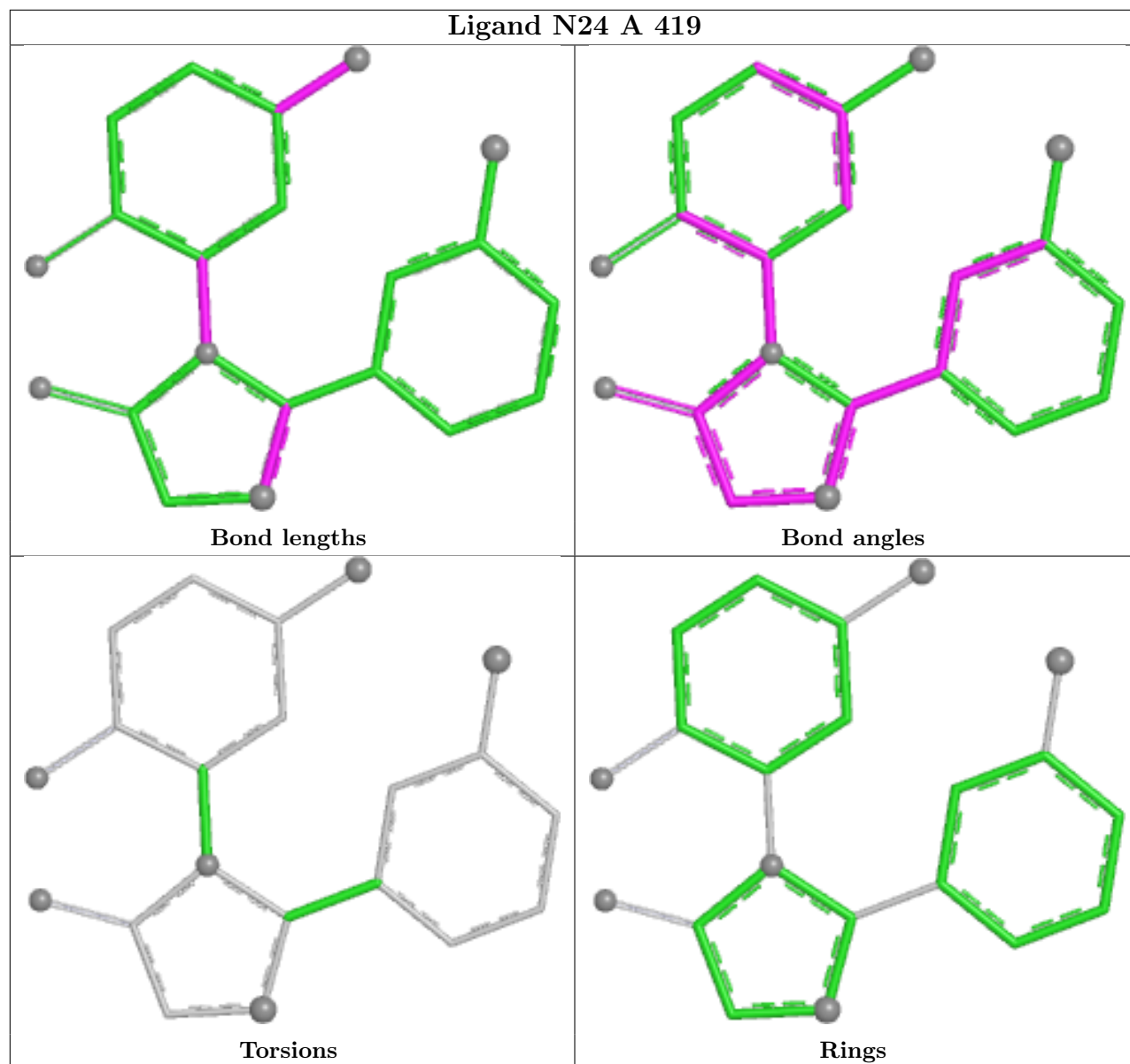
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	419	N24	3	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%)	0.69	35 (8%) 15 12	33, 62, 107, 124	0
2	B	196/394 (49%)	1.58	60 (30%) 1 1	45, 79, 123, 130	0
3	C	341/372 (91%)	0.40	11 (3%) 50 41	24, 56, 92, 117	0
4	D	281/300 (93%)	0.50	14 (4%) 34 27	34, 61, 95, 108	0
5	E	174/178 (97%)	1.16	24 (13%) 6 5	54, 82, 119, 130	0
6	F	167/168 (99%)	0.31	9 (5%) 31 23	37, 53, 77, 104	0
7	G	137/151 (90%)	1.62	43 (31%) 1 1	33, 101, 120, 137	0
All	All	1695/1981 (85%)	0.79	196 (11%) 9 7	24, 64, 114, 137	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	54	ALA	6.1
7	G	28	GLU	5.3
2	B	349	ARG	5.3
3	C	201	SER	5.3
2	B	174	SER	5.1
4	D	207	LEU	5.1
7	G	63	PRO	4.7
2	B	172	GLY	4.5
2	B	173	PHE	4.5
7	G	9	ALA	4.4
7	G	55	LEU	4.3
2	B	184	ILE	4.3
2	B	154	GLY	4.2
1	A	353	LEU	4.2
7	G	150	THR	4.1
2	B	178	LEU	4.0
1	A	415	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	345	GLU	4.0
3	C	372	VAL	3.9
1	A	161	ARG	3.9
2	B	333	ASP	3.9
7	G	30	GLY	3.8
7	G	58	ALA	3.8
6	F	57	GLU	3.8
2	B	290	ASP	3.8
2	B	291	ILE	3.8
1	A	158	VAL	3.7
7	G	11	PHE	3.7
7	G	95	VAL	3.7
2	B	162	GLY	3.5
2	B	206	HIS	3.5
7	G	52	THR	3.4
3	C	202	CYS	3.4
7	G	121	SER	3.4
1	A	159	GLY	3.4
7	G	24	PHE	3.4
1	A	414	PHE	3.3
1	A	262	ILE	3.3
2	B	329	VAL	3.3
2	B	332	GLY	3.3
7	G	17	GLY	3.3
1	A	82	ILE	3.2
7	G	80	LEU	3.2
6	F	92	ARG	3.2
7	G	39	GLU	3.2
4	D	108	SER	3.2
7	G	25	VAL	3.2
2	B	189	ILE	3.2
5	E	2	PRO	3.2
2	B	346	ASP	3.1
2	B	186	GLY	3.1
1	A	81	GLY	3.1
2	B	322	LYS	3.1
2	B	288	ALA	3.0
2	B	167	CYS	3.0
6	F	58	LYS	3.0
2	B	181	ARG	3.0
5	E	164	VAL	3.0
2	B	166	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	297	PHE	2.9
7	G	42	VAL	2.9
7	G	64	ILE	2.9
7	G	87	LYS	2.9
5	E	39	THR	2.8
7	G	66	THR	2.8
5	E	124	GLN	2.8
5	E	62	ASN	2.8
5	E	85	CYS	2.8
2	B	180	ARG	2.8
2	B	169	VAL	2.8
7	G	53	ALA	2.8
7	G	60	LYS	2.8
1	A	221	LEU	2.7
2	B	286	ILE	2.7
7	G	94	ALA	2.7
4	D	212	THR	2.7
7	G	50	ASN	2.7
2	B	185	ALA	2.7
1	A	371	HIS	2.7
2	B	190	THR	2.7
7	G	27	GLU	2.7
2	B	182	LEU	2.7
1	A	261	ALA	2.6
1	A	264	LYS	2.6
2	B	278	VAL	2.6
7	G	88	ALA	2.6
1	A	156	ARG	2.6
1	A	352	GLU	2.6
2	B	342	ILE	2.6
4	D	205	PRO	2.6
1	A	265	LYS	2.6
1	A	400	TYR	2.6
2	B	327	GLU	2.6
6	F	31	GLU	2.6
6	F	3	ALA	2.6
7	G	122	SER	2.5
1	A	360	PRO	2.5
3	C	288	PRO	2.5
2	B	230	GLU	2.5
2	B	294	ARG	2.5
1	A	354	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	104	PRO	2.5
2	B	163	VAL	2.5
7	G	91	ILE	2.5
1	A	218	GLU	2.5
2	B	287	GLN	2.5
2	B	295	SER	2.5
7	G	59	LEU	2.5
7	G	12	ARG	2.5
1	A	52	MET	2.4
2	B	330	LEU	2.4
4	D	177	ILE	2.4
1	A	359	LYS	2.4
2	B	298	TYR	2.4
2	B	281	LEU	2.4
4	D	206	PRO	2.4
3	C	200	SER	2.4
7	G	44	SER	2.4
2	B	177	HIS	2.4
1	A	172	ASP	2.4
7	G	23	LYS	2.4
6	F	101	PHE	2.4
3	C	319	ALA	2.4
5	E	142	LEU	2.4
2	B	277	GLY	2.4
7	G	36	GLY	2.4
2	B	183	ASP	2.4
1	A	26	GLU	2.4
1	A	68	GLU	2.4
2	B	289	ALA	2.4
3	C	75	ASN	2.3
3	C	142	ARG	2.3
2	B	285	THR	2.3
2	B	324	LEU	2.3
5	E	36	THR	2.3
1	A	39	GLU	2.3
7	G	26	ASP	2.3
5	E	24	ILE	2.3
7	G	47	ARG	2.3
7	G	82	VAL	2.3
5	E	103	PHE	2.3
2	B	325	TYR	2.3
5	E	117	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	265	LEU	2.3
2	B	323	GLN	2.3
2	B	326	LEU	2.3
1	A	79	ARG	2.3
5	E	146	GLU	2.2
5	E	105	ILE	2.2
5	E	151	PRO	2.2
3	C	175	GLU	2.2
5	E	121	ALA	2.2
2	B	176	PRO	2.2
5	E	88	LYS	2.2
1	A	91	ARG	2.2
7	G	97	SER	2.2
4	D	228	PHE	2.2
7	G	93	LYS	2.2
2	B	282	LEU	2.2
4	D	209	LEU	2.2
1	A	363	ILE	2.2
5	E	94	GLU	2.2
5	E	12	ASP	2.1
7	G	51	MET	2.1
4	D	158	LYS	2.1
5	E	58	TYR	2.1
2	B	344	ILE	2.1
1	A	227	VAL	2.1
5	E	81	LYS	2.1
3	C	251	THR	2.1
6	F	102	PHE	2.1
6	F	168	PHE	2.1
2	B	187	ARG	2.1
1	A	160	GLU	2.1
1	A	220	SER	2.1
7	G	56	GLN	2.1
7	G	120	ASN	2.1
2	B	170	TYR	2.1
4	D	170	LYS	2.1
5	E	169	MET	2.1
7	G	37	PRO	2.1
2	B	292	ASP	2.1
2	B	293	THR	2.1
1	A	229	GLU	2.1
2	B	284	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	192	SER	2.0
4	D	231	HIS	2.0
5	E	89	SER	2.0
6	F	27	SER	2.0
2	B	321	LEU	2.0
3	C	183	THR	2.0
1	A	85	ASP	2.0
1	A	266	GLU	2.0
4	D	107	ASP	2.0
4	D	213	ASP	2.0
5	E	154	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

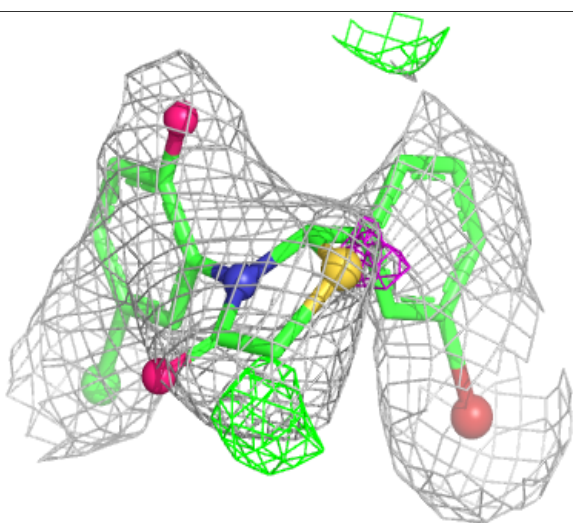
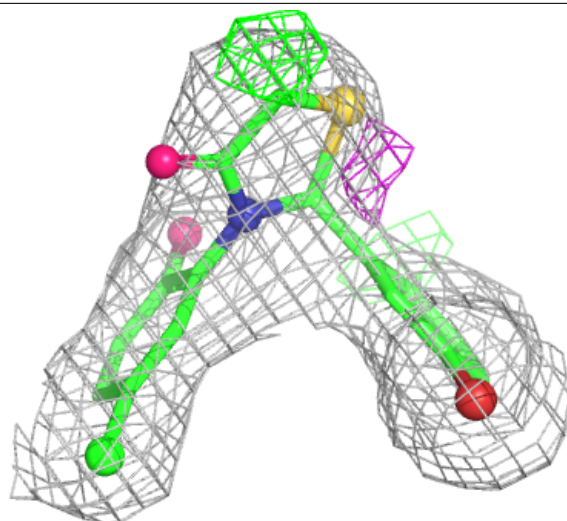
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	N24	A	419	21/21	0.92	0.15	87,90,92,93	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 N24 A 419:

$2mF_o-DF_c$ (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.