



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 08:12 PM EDT

PDB ID : 3DXM
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 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 : 2.27
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) : 2.27

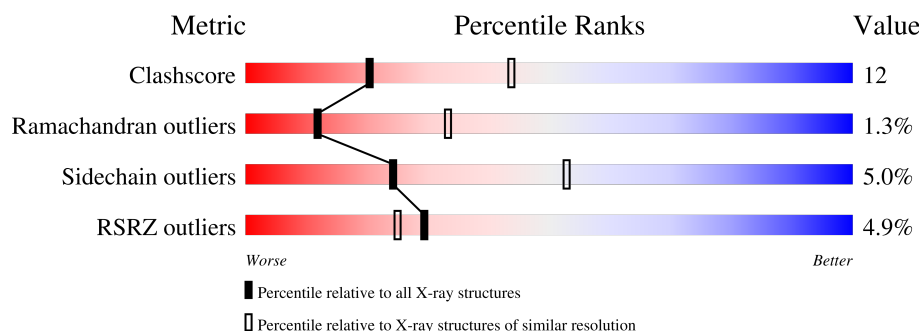
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div> </div>
2	B	394	<div> <div>4%</div> <div> <div></div> <div>30%</div> <div>15%</div> <div>•</div> <div>50%</div> </div> </div>
3	C	372	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>• 8%</div> </div> </div>
4	D	300	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
5	E	178	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>5%</div> <div>•</div> </div> </div>
6	F	168	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>•••</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G	151	<div><div></div><div>15%</div><div>70%</div><div>19%</div><div>•</div><div>9%</div></div>

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			

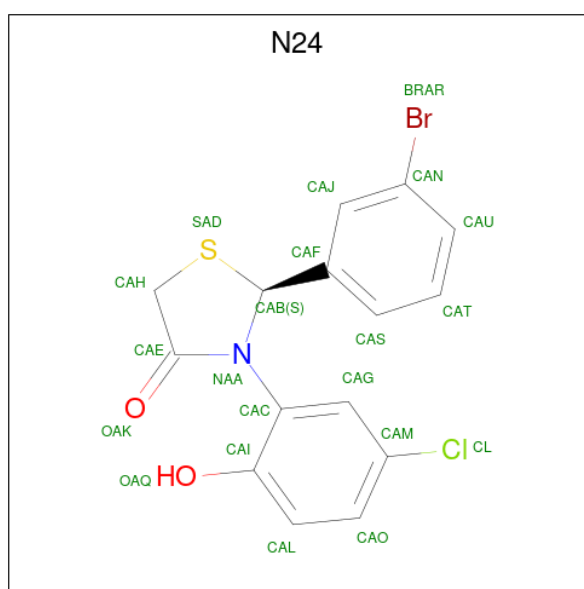
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

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 (three-letter code: 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		

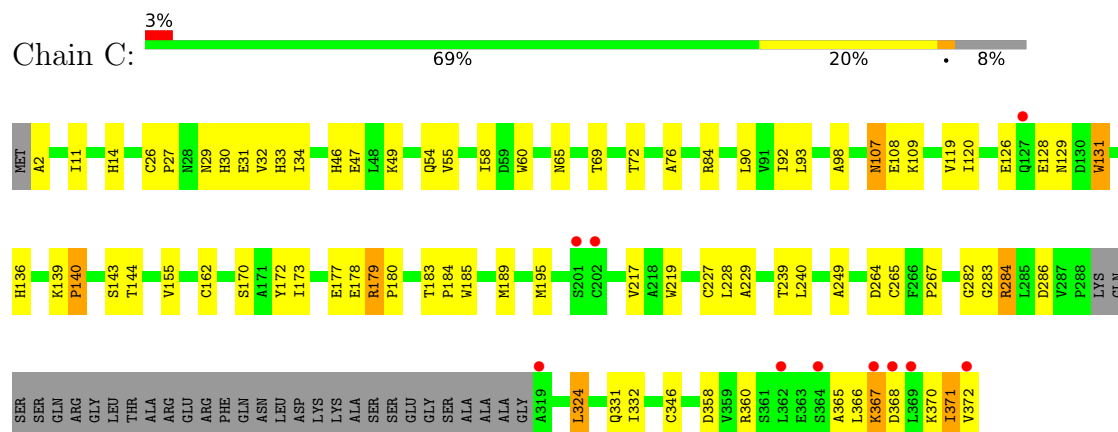
Continued on next page...

Continued from previous page...

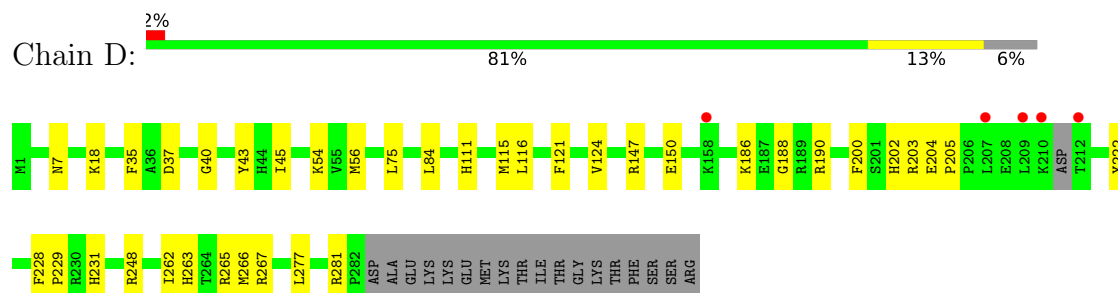
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	10	Total	O	0	0
			10	10		
9	G	1	Total	O	0	0
			1	1		

GLU
TYR
GLN
GLY
VAL
ARG
VAL
GLU
LYS
LEU
GLY
THR
VAL
ARG

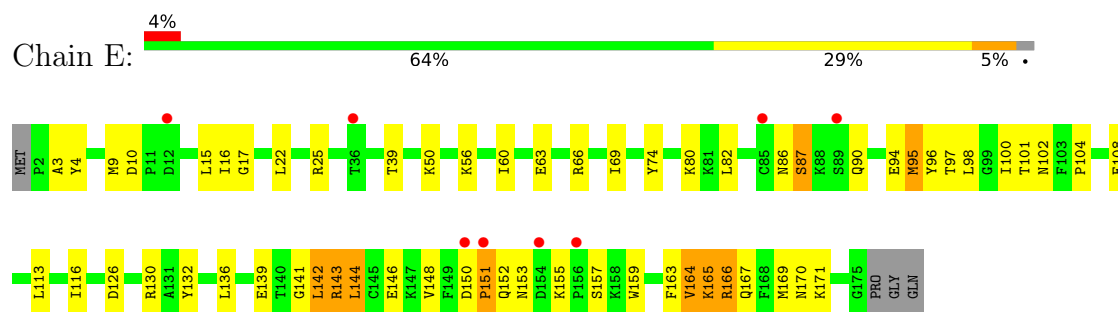
• Molecule 3: Actin-related protein 2/3 complex subunit 1B



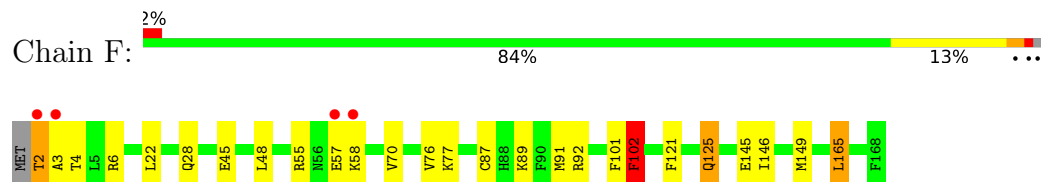
• Molecule 4: Actin-related protein 2/3 complex subunit 2



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

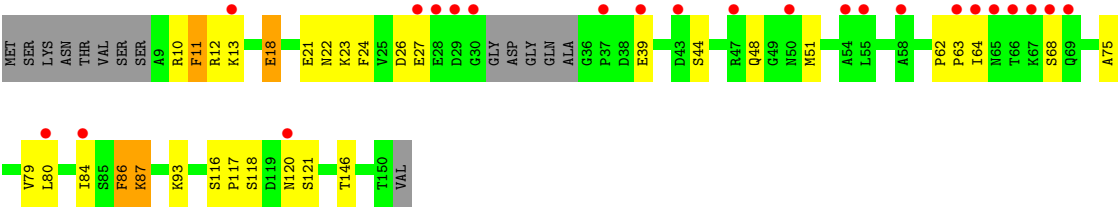


• Molecule 6: Actin-related protein 2/3 complex subunit 4



• 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 39.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.85) 90.2 (39.53-2.80)	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 0.241 , (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)	0.31 , 41.6	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	0.31	0/3280	0.64	4/4450 (0.1%)
2	B	0.32	0/1555	0.61	1/2110 (0.0%)
3	C	0.29	0/2718	0.64	2/3689 (0.1%)
4	D	0.28	0/2319	0.54	0/3129
5	E	0.28	0/1433	0.60	2/1934 (0.1%)
6	F	0.30	0/1393	0.58	1/1868 (0.1%)
7	G	0.28	0/1056	0.54	0/1420
All	All	0.30	0/13754	0.60	10/18600 (0.1%)

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	166	ARG	N-CA-C	-6.26	94.10	111.00
1	A	80	HIS	N-CA-C	-6.10	94.53	111.00
1	A	83	VAL	N-CA-C	5.97	127.11	111.00
3	C	11	ILE	N-CA-C	-5.96	94.89	111.00
1	A	78	ILE	CB-CA-C	-5.71	100.17	111.60
3	C	283	GLY	N-CA-C	5.39	126.57	113.10
2	B	301	ILE	N-CA-C	-5.33	96.62	111.00
1	A	85	ASP	N-CA-C	-5.30	96.69	111.00
6	F	102	PHE	N-CA-C	5.14	124.89	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	17	GLY	N-CA-C	-5.06	100.46	113.10

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3199	0	3149	89	0
2	B	1525	0	1513	73	0
3	C	2649	0	2604	67	0
4	D	2271	0	2243	28	0
5	E	1400	0	1394	44	0
6	F	1371	0	1410	27	0
7	G	1044	0	1052	23	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	334	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 12.

All (334) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:169:VAL:HG13	2:B:173:PHE:C	2.08	0.74
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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:107:ASN:C	3:C:107:ASN:HD22	2.01	0.64
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: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
2:B:302:VAL:C	2:B:303:LEU:HD23	2.19	0.63
3:C:189:MET:HG2	3:C:195:MET:HE3	1.80	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
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
3:C:107:ASN:HD22	3:C:108:GLU:N	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
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: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
1:A:246:ASP:OD1	5:E:50:LYS:HE3	2.01	0.60
3:C:365:ALA:C	3:C:366:LEU:HD12	2.22	0.59
1:A:289:ASN:HD22	1:A:289:ASN:C	2.06	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
5:E:60:ILE:HD13	5:E:66:ARG:HG2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:146:ILE:HA	6:F:149:MET:HE2	1.84	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:190:ILE:C	1:A:191:LYS:HD3	2.25	0.57
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
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:371:ILE:O	3:C:372:VAL:HB	2.05	0.56
5:E:150:ASP:C	5:E:152:GLN:H	2.08	0.56
1:A:84:GLU:HG3	1:A:86:TRP:HE1	1.69	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
6:F:2:THR:C	6:F:4:THR:H	2.09	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
2:B:299:LYS:HA	2:B:343:ARG:O	2.07	0.55
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.38	0.54
2:B:170:TYR:O	2:B:171:GLU:C	2.45	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
5:E:113:LEU:HD11	5:E:169:MET:HE3	1.89	0.54
7:G:18:GLU:OE1	7:G:23:LYS:NZ	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD12	1:A:82:ILE:O	2.07	0.54
1:A:194:PRO:C	1:A:195:ILE:HD12	2.28	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
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
3:C:172:TYR:OH	3:C:179:ARG:HD2	2.08	0.53
1:A:111:LEU:HD23	1:A:111:LEU:C	2.29	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
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.43	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
4:D:248:ARG:HD3	4:D:248:ARG:C	2.30	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
5:E:150:ASP:C	5:E:152:GLN:N	2.63	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:126:GLU:C	3:C:128:GLU:H	2.13	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
5:E:165:LYS:O	5:E:165:LYS:HG2	2.09	0.51
1:A:176:HIS:CD2	1:A:192:HIS:HD2	2.27	0.50
5:E:95:MET:HA	5:E:95:MET:HE2	1.92	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:323:GLN:CD	7:G:12:ARG:HA	2.32	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:173:PHE:CG	2:B:174:SER:N	2.79	0.50
1:A:82:ILE:HD12	1:A:82:ILE:C	2.33	0.49
2:B:163:VAL:HG22	2:B:164:THR:N	2.26	0.49
3:C:228:LEU:C	3:C:228:LEU:HD23	2.33	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
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:189:MET:HG2	3:C:195:MET:CE	2.42	0.49
2:B:326:LEU:HD23	2:B:326:LEU:C	2.33	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
2:B:330:LEU:C	2:B:332:GLY:H	2.17	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
3:C:367:LYS:HD3	3:C:367:LYS:C	2.33	0.48
4:D:188:GLY:HA3	6:F:165:LEU:HD23	1.95	0.48
5:E:69:ILE:CG2	5:E:169:MET:HE1	2.43	0.48
5:E:69:ILE:HG23	5:E:169:MET:HE1	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
3:C:107:ASN:ND2	3:C:107:ASN:C	2.67	0.47
2:B:180:ARG:HB2	2:B:281:LEU:HD21	1.94	0.47
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:239:VAL:HG23	1:A:240:LYS:N	2.29	0.47
3:C:170:SER:HB2	3:C:195:MET:HE3	1.96	0.47
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.97	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
3:C:178:GLU:O	3:C:179:ARG:C	2.54	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
6:F:146:ILE:HA	6:F:149:MET:HE3	1.99	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
5:E:50:LYS:NZ	5:E:159:TRP:O	2.49	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
5:E:95:MET:HG2	5:E:141:GLY:C	2.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.83	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
1:A:262:ILE:O	1:A:263:SER:OG	2.33	0.42
3:C:69:THR:O	3:C:76:ALA:HA	2.20	0.42
4:D:75:LEU:HD23	4:D:75:LEU:C	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:228:PHE:H	4:D:231:HIS:CD2	2.32	0.42
1:A:76:TRP:C	1:A:78:ILE:H	2.22	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
1:A:311:VAL:C	1:A:314:PRO:HD2	2.40	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:156:VAL:HA	2:B:302:VAL:O	2.20	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
5:E:164:VAL:HG22	5:E:164:VAL:O	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
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
1:A:217:PRO:C	1:A:219:GLN:H	2.25	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
1:A:329:ARG:O	1:A:330:ASP:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:76:VAL:HG12	6:F:77:LYS:N	2.37	0.40
1:A:135:ASN:HB3	1:A:397:LYS:HZ2	1.87	0.40
4:D:263:HIS:O	4:D:267:ARG:HG3	2.22	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%)	12	33
2	B	194/394 (49%)	164 (84%)	22 (11%)	8 (4%)	3	9
3	C	337/372 (91%)	317 (94%)	19 (6%)	1 (0%)	41	68
4	D	277/300 (92%)	273 (99%)	4 (1%)	0	100	100
5	E	172/178 (97%)	161 (94%)	7 (4%)	4 (2%)	6	20
6	F	165/168 (98%)	159 (96%)	4 (2%)	2 (1%)	13	35
7	G	133/151 (88%)	126 (95%)	5 (4%)	2 (2%)	10	30
All	All	1671/1981 (84%)	1570 (94%)	79 (5%)	22 (1%)	12	33

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	336 (96%)	14 (4%)	31	62
2	B	161/345 (47%)	144 (89%)	17 (11%)	6	18
3	C	290/313 (93%)	280 (97%)	10 (3%)	37	67
4	D	247/264 (94%)	241 (98%)	6 (2%)	49	77
5	E	153/159 (96%)	141 (92%)	12 (8%)	12	32
6	F	154/155 (99%)	149 (97%)	5 (3%)	39	69
7	G	112/123 (91%)	103 (92%)	9 (8%)	12	31
All	All	1467/1722 (85%)	1394 (95%)	73 (5%)	24	53

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	19	LEU
1	A	68	GLU
1	A	71	THR
1	A	143	VAL
1	A	191	LYS
1	A	230	ARG
1	A	251	LYS
1	A	255	GLN
1	A	289	ASN
1	A	310	ASP
1	A	343	VAL
1	A	353	LEU
1	A	363	ILE
2	B	171	GLU
2	B	175	LEU
2	B	182	LEU
2	B	184	ILE
2	B	200	ARG
2	B	220	LEU
2	B	274	GLU
2	B	290	ASP
2	B	297	PHE
2	B	299	LYS
2	B	303	LEU
2	B	320	GLU
2	B	337	LEU
2	B	338	SER
2	B	340	PHE
2	B	342	ILE
2	B	346	ASP
3	C	30	HIS
3	C	90	LEU
3	C	92	ILE
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	179	ARG
3	C	284	ARG
3	C	324	LEU
3	C	367	LYS
4	D	18	LYS
4	D	54	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	25	ARG
5	E	39	THR
5	E	80	LYS
5	E	95	MET
5	E	142	LEU
5	E	143	ARG
5	E	144	LEU
5	E	146	GLU
5	E	165	LYS
5	E	166	ARG
6	F	2	THR
6	F	6	ARG
6	F	101	PHE
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
7	G	68	SER
7	G	86	PHE
7	G	87	LYS
7	G	120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) 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	305	GLN
1	A	306	ASN
1	A	318	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	370	HIS
1	A	371	HIS
1	A	395	HIS
2	B	205	ASN
2	B	231	GLN
2	B	267	GLN
2	B	284	ASN
2	B	323	GLN
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	112	GLN
4	D	140	ASN
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
5	E	102	ASN
6	F	28	GLN
6	F	125	GLN
7	G	22	ASN
7	G	61	ASN
7	G	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	N24	A	419	-	23,23,23	1.74	3 (13%)	30,33,33	1.72	7 (23%)

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	-5.57	1.36	1.43
8	A	419	N24	CAB-SAD	-3.88	1.79	1.84
8	A	419	N24	CAM-CL	2.51	1.80	1.74

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	419	N24	CAH-CAE-NAA	4.93	115.52	112.14
8	A	419	N24	CAE-CAH-SAD	-4.01	104.17	107.60
8	A	419	N24	CAF-CAB-SAD	2.64	115.53	111.62
8	A	419	N24	CAH-SAD-CAB	2.48	96.90	93.14
8	A	419	N24	CAF-CAJ-CAN	2.37	121.40	119.56
8	A	419	N24	OAK-CAE-CAH	-2.17	118.94	123.54
8	A	419	N24	CAO-CAM-CAG	-2.15	118.67	121.53

There are no chirality outliers.

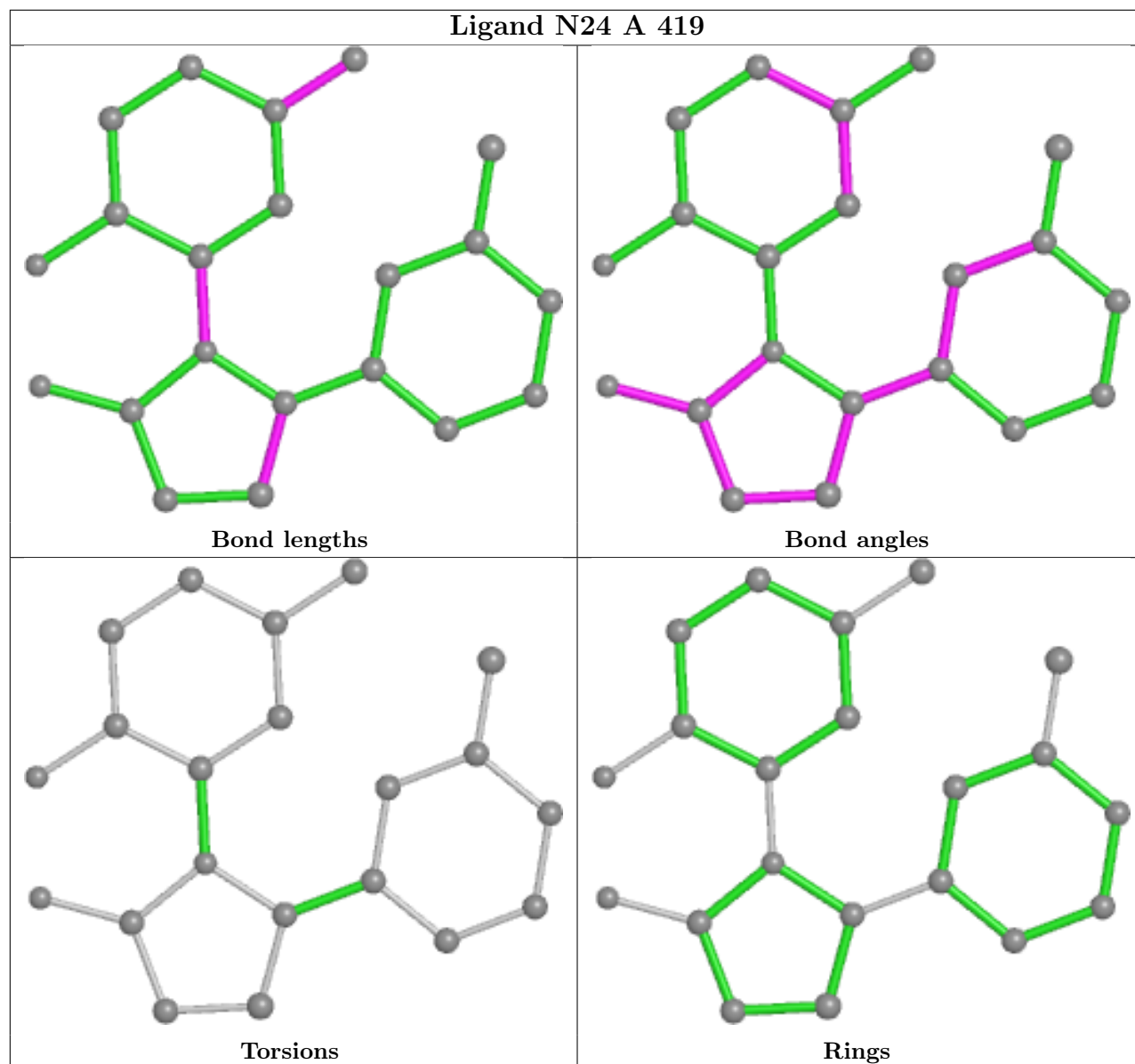
There are no torsion outliers.

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%)	0.17	19 (4%) 30 26	33, 62, 107, 124	0
2	B	196/394 (49%)	0.50	14 (7%) 16 12	45, 79, 123, 130	0
3	C	341/372 (91%)	0.06	10 (2%) 51 47	24, 56, 92, 117	0
4	D	281/300 (93%)	-0.07	5 (1%) 68 66	34, 61, 95, 108	0
5	E	174/178 (97%)	0.25	8 (4%) 32 27	54, 82, 119, 130	0
6	F	167/168 (99%)	-0.15	4 (2%) 59 56	37, 53, 77, 104	0
7	G	137/151 (90%)	0.77	23 (16%) 1 1	33, 101, 120, 137	0
All	All	1695/1981 (85%)	0.17	83 (4%) 29 25	24, 64, 114, 137	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	372	VAL	6.0
2	B	173	PHE	5.7
2	B	174	SER	5.3
7	G	54	ALA	5.1
7	G	63	PRO	4.8
3	C	201	SER	4.6
1	A	156	ARG	4.3
1	A	161	ARG	4.3
1	A	51	VAL	4.2
2	B	178	LEU	4.2
1	A	266	GLU	4.1
7	G	55	LEU	4.0
7	G	27	GLU	4.0
7	G	28	GLU	3.9
5	E	85	CYS	3.7
1	A	81	GLY	3.7
1	A	351	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	359	LYS	3.7
1	A	82	ILE	3.6
1	A	352	GLU	3.5
3	C	369	LEU	3.5
1	A	39	GLU	3.4
7	G	39	GLU	3.4
3	C	367	LYS	3.4
7	G	64	ILE	3.4
7	G	67	LYS	3.3
1	A	415	GLY	3.2
7	G	66	THR	3.2
7	G	50	ASN	3.2
3	C	202	CYS	3.2
7	G	58	ALA	3.2
5	E	151	PRO	3.0
2	B	332	GLY	3.0
4	D	212	THR	2.9
4	D	210	LYS	2.9
7	G	68	SER	2.9
5	E	12	ASP	2.9
1	A	52	MET	2.9
2	B	181	ARG	2.9
3	C	368	ASP	2.9
6	F	3	ALA	2.8
7	G	37	PRO	2.7
7	G	47	ARG	2.7
4	D	207	LEU	2.7
5	E	89	SER	2.7
6	F	58	LYS	2.7
7	G	29	ASP	2.7
3	C	319	ALA	2.7
5	E	150	ASP	2.6
6	F	2	THR	2.6
2	B	295	SER	2.6
3	C	364	SER	2.5
6	F	57	GLU	2.5
7	G	69	GLN	2.5
7	G	65	ASN	2.5
2	B	154	GLY	2.5
5	E	154	ASP	2.5
1	A	348	LYS	2.4
1	A	349	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	43	ASP	2.4
5	E	156	PRO	2.4
7	G	30	GLY	2.4
1	A	157	GLN	2.3
1	A	264	LYS	2.3
4	D	209	LEU	2.3
2	B	172	GLY	2.3
3	C	127	GLN	2.3
7	G	13	LYS	2.3
3	C	362	LEU	2.2
2	B	184	ILE	2.2
1	A	414	PHE	2.2
2	B	290	ASP	2.2
7	G	120	ASN	2.2
5	E	36	THR	2.1
7	G	84	ILE	2.1
2	B	330	LEU	2.1
1	A	416	VAL	2.1
4	D	158	LYS	2.1
1	A	158	VAL	2.1
2	B	345	GLU	2.1
2	B	334	VAL	2.0
7	G	80	LEU	2.0
2	B	183	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](#)

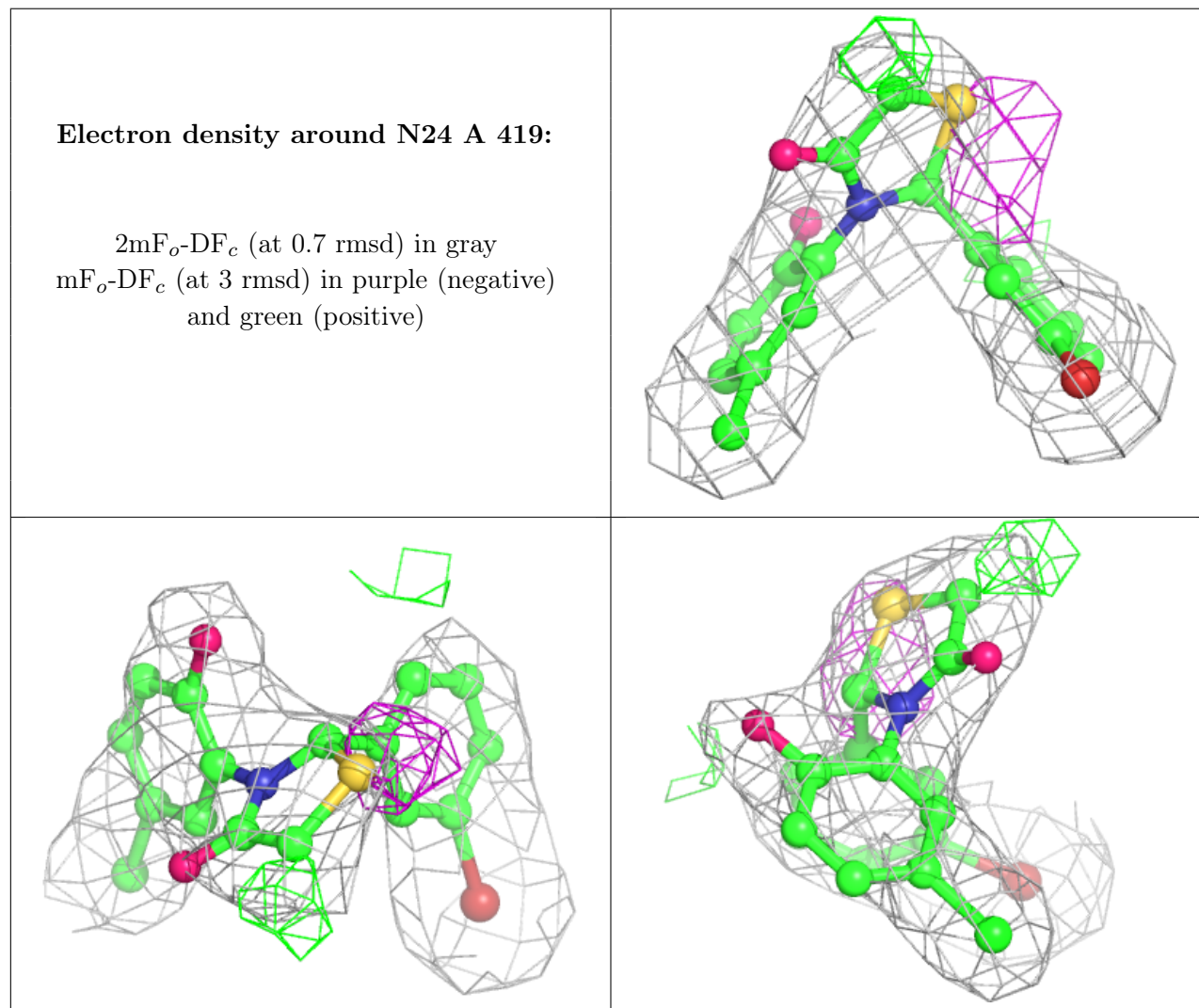
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
8	N24	A	419	21/21	0.92	0.21	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.