Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 06:29 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 (i) 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 (i)) were used in the production of this report:

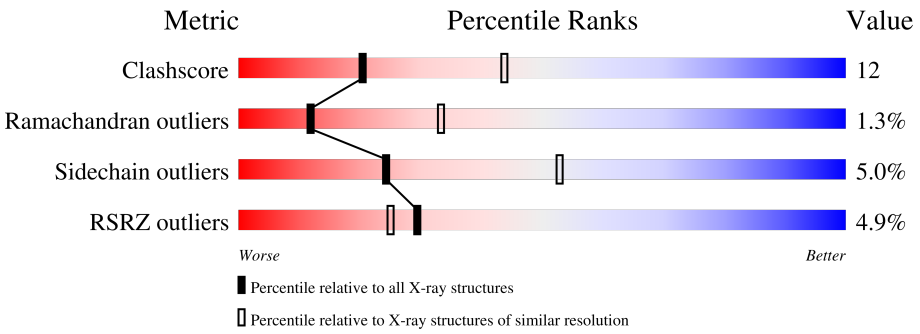
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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

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Mol	Chain	Length	Quality of chain
7	G	151	15% 70% 19% • 9%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	399	3199	2055	534	595	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	196	1525	980	258	283	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	341	2649	1681	464	485	19	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	281	2271	1445	394	424	8	0	0	0

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

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

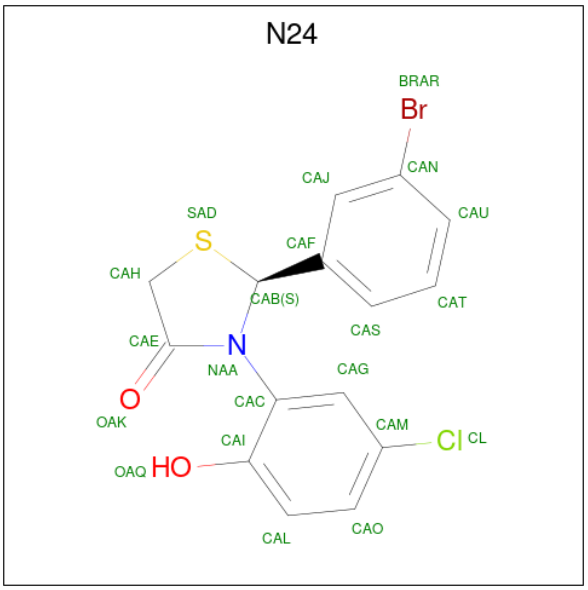
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

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

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

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

- Molecule 8 is (2S)-2-(3-bromophenyl)-3-(5-chloro-2-hydroxyphenyl)-1,3-thiazolidin-4-one (three-letter code: N24) (formula: $C_{15}H_{11}BrClNO_2S$).



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

- Molecule 9 is water.

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

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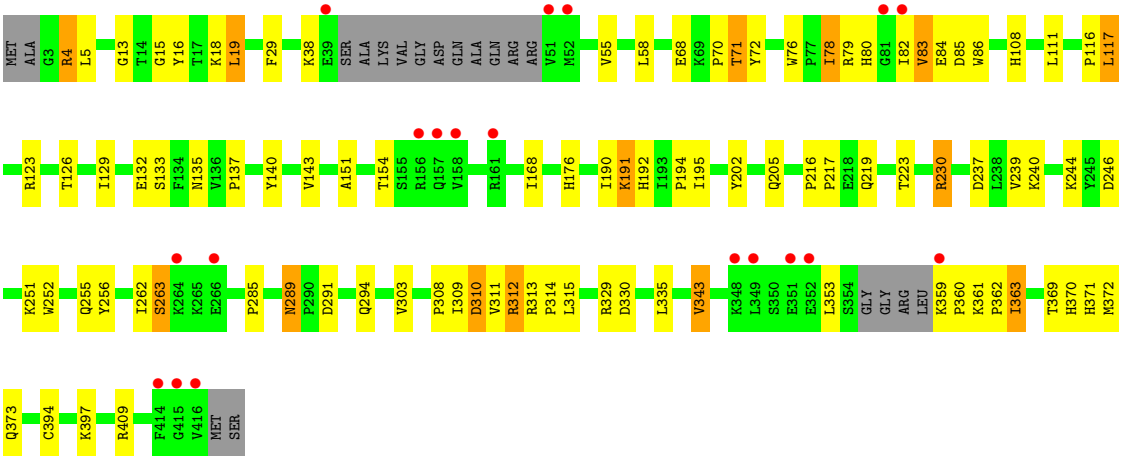
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	F	10	10	10	0	0
			Total	O		
9	G	1	1	1	0	0

3 Residue-property plots (i)

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

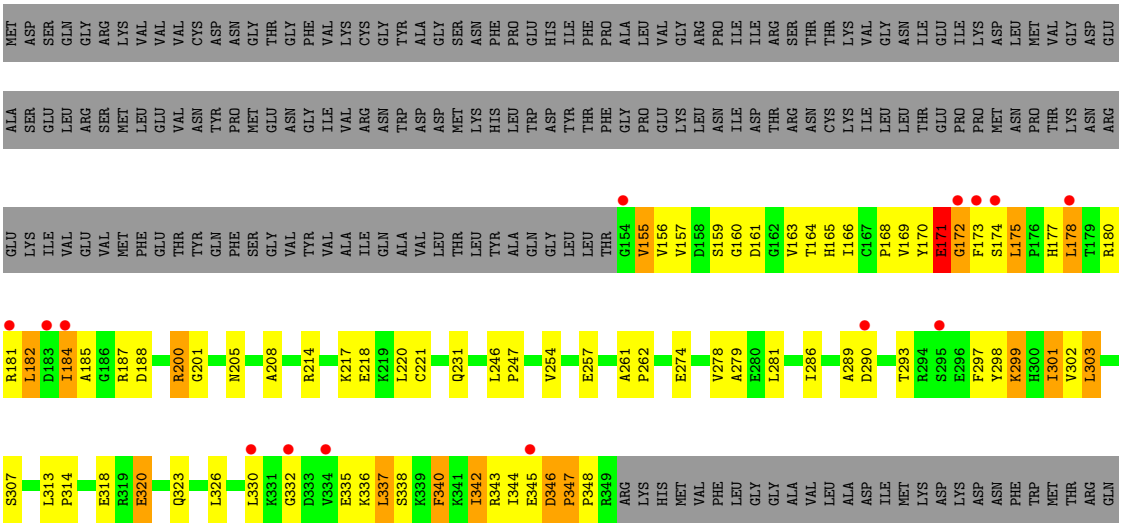
- Molecule 1: Actin-related protein 3

Chain A:



- Molecule 2: Actin-related protein 2

Chain B:



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

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

Chain C:

MET A2 I11 H14 C26 P27 N28 N29 H30 E31 V32 H33 I34 H46 E47 L48 K49 Q54 V55 I58 D59 W60 N65 T69 T72 A76 R84 L90 V91 I92 L93 A98 N107 E108 K109 V119 I120 E126 Q127 E128 N129 D130 W131

H136 K139 P140 S143 T144 V155 C162 S170 A171 Y172 I173 E177 E178 R179 P180 T183 P184 W185 M189 M195 S201 C202 V217 A218 W219 C227 L228 A229 T239 L240 A249 D264 C265 F266 P267 G282 G283 R284 L285 D286 V287 P288 LYS GLN

SER SER GLN ARG GLY LEU THR ALA ARG GLU ARG PHE GLN ASN LEU ASP LYS LYS ALA SER SER GLU GLY SER ALA ALA ALA GLY A319 L324 Q331 I332 C346 D358 V359 R360 S361 L362 E363 S364 A365 L366 K367 D368 L369 K370 I371 V372

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

Chain D:

M1 N7 K18 F35 A36 D37 G40 Y43 H44 I45 K54 V55 M56 L75 L84 H111 M115 L116 F121 V124 R147 E150 K158 K186 E187 G188 R189 R190 F200 S201 H202 R203 E204 P205 P206 L207 E208 L209 K210 ASP T212 Y222

F228 P229 R230 H231 R248 I262 H263 T264 R265 M266 R267 L277 R281 P282 ASP ALA GLU LYS LYS GLU MET LYS THR ILE THR GLY LYS THR PHE SER SER ARG

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

Chain E:

MET P2 A3 Y4 M9 D10 P11 D12 L15 I16 G17 L22 R25 T36 T39 K50 K56 I60 E63 R66 I69 Y74 K80 K81 L82 C85 N86 S87 K88 S89 Q90 E94 M95 Y96 T97 L98 G99 I100 T101 N102 F103 P104 E108

L113 I116 D126 R130 A131 Y132 L136 E139 T140 G141 L142 R143 L144 C145 E146 K147 V148 F149 D150 P151 Q152 N153 D154 K155 P156 S157 K158 W159 F163 V164 K165 R166 Q167 F168 M169 N170 K171 G175 PRO GLY GLN

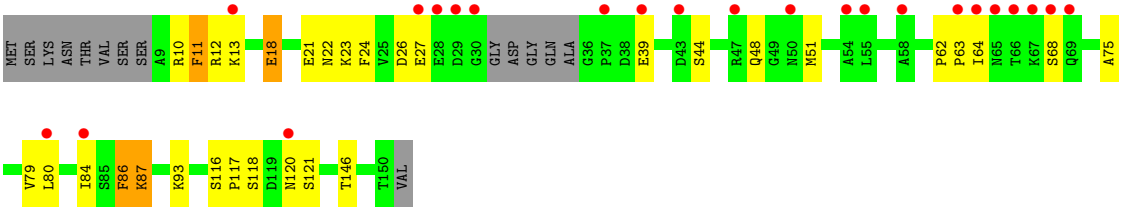
- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:

MET T2 A3 T4 L5 R6 L22 Q28 E45 L48 R55 N56 E57 K58 V70 V76 K77 C87 H88 K89 F90 M91 R92 F101 F102 F121 Q125 E145 I146 M149 L165 F168

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

Chain G:


MET SER LYS ASN THR VAL SER SER A9 R10 F11 R12 K13 E18 E21 N22 K23 F24 V25 D26 E27 E28 D29 G30 GLY ASP GLY GLN ALA G36 P37 D38 E39 D43 S44 R47 Q48 G49 N50 M51 A54 L55 A58 P62 P63 I64 N65 T66 K67 S68 Q69 A75
V79 L80 I84 S85 F86 K87 K93 S116 P117 S118 D119 N120 S121 T146 T150 VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.38Å 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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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 (i)

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

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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

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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

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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 (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 monosaccharides 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	1.74	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(^{o})	Ideal(^{o})
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.

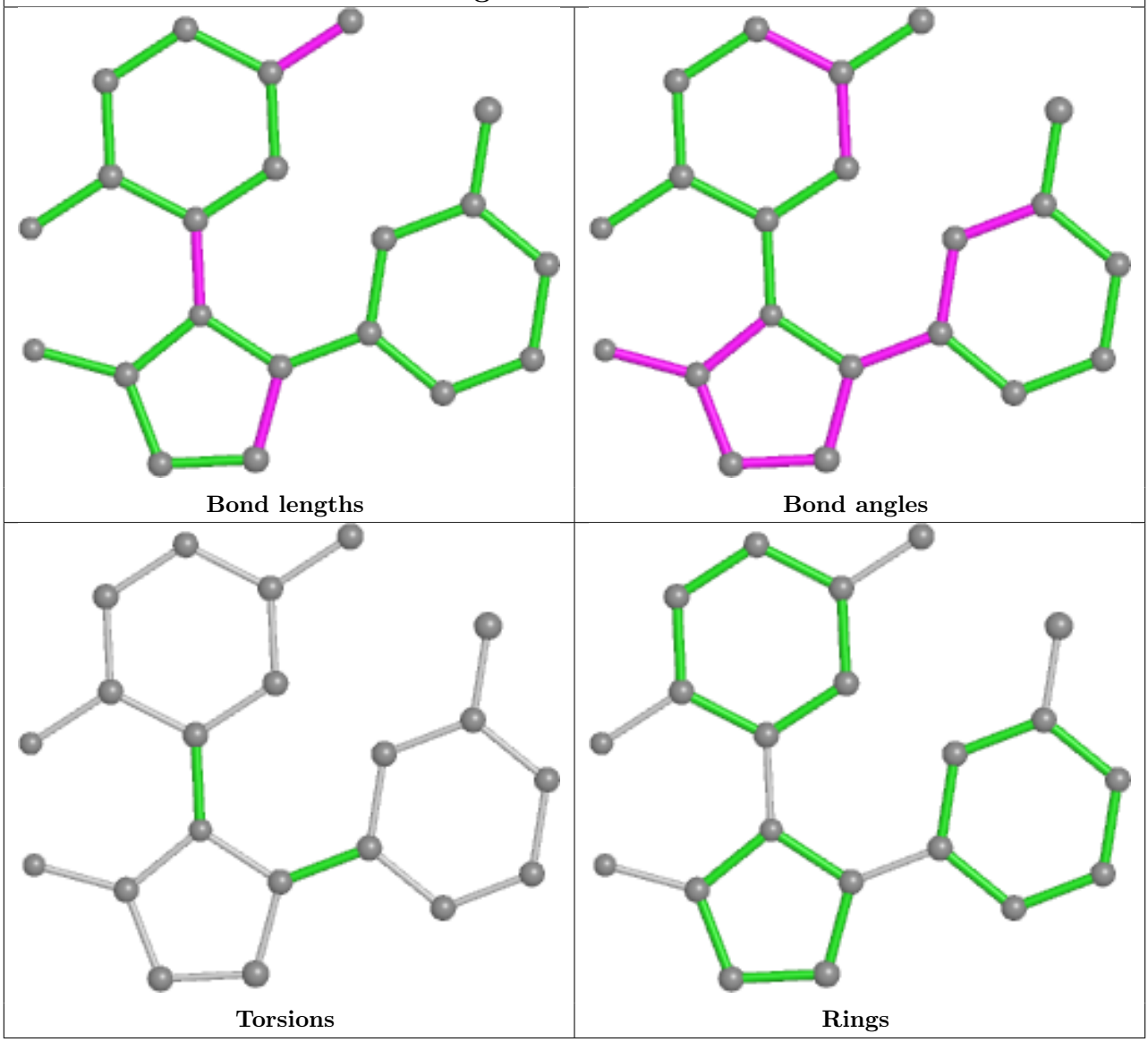
There are no ring outliers.

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 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 N24 A 419



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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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

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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)

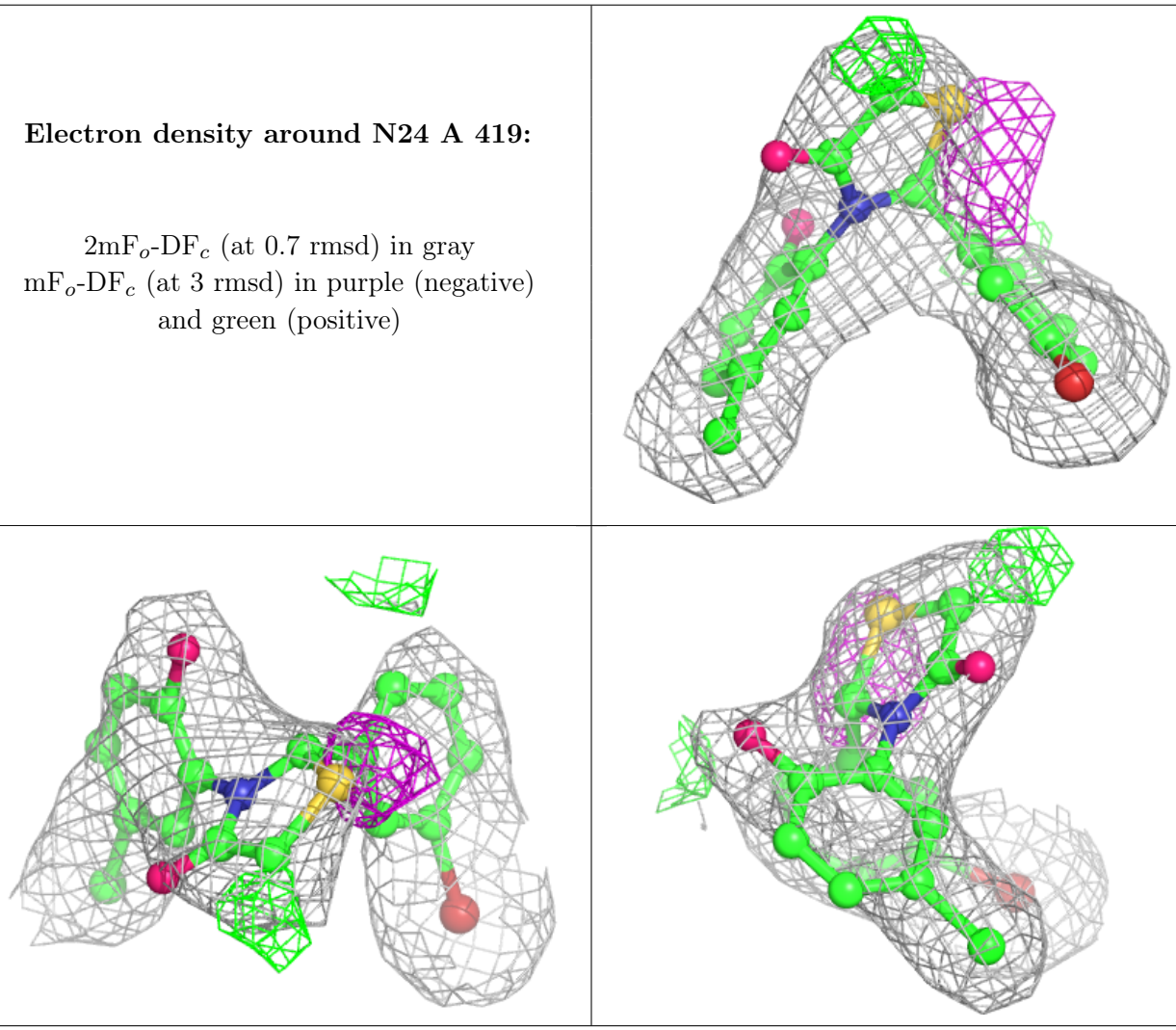
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^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.

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.