Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 04:10 PM EDT

PDB ID	:	1XPO
Title	:	Structural mechanism of inhibition of the Rho transcription termination factor by the antibiotic bicyclomycin
Authors	:	Skordalakes, E.; Brogan, A.P.; Park, B.S.; Kohn, H.; Berger, J.M.
Deposited on	:	2004-10-09
Resolution	:	3.15 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:

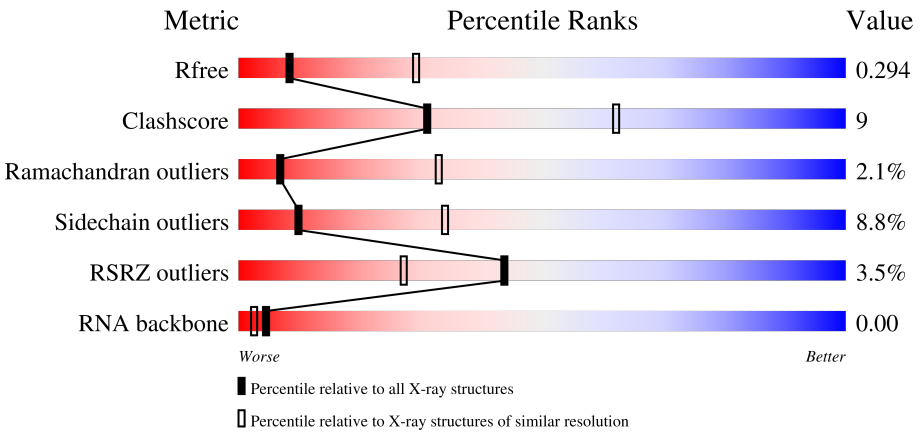
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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	G	8	25% 12% 12% 75%
1	H	8	12% 12% 12% 75%
1	J	8	12% 12% 12% 75%
1	K	8	25% 12% 12% 75%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	8	12% 12% 12% 75%
1	M	8	25% 12% 12% 75%
2	A	419	4% 68% 26%
2	B	419	5% 62% 33%
2	C	419	3% 71% 22%
2	D	419	% 70% 22% 5%
2	E	419	3% 68% 26%
2	F	419	2% 73% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AGS	C	3600	-	-	-	X
4	AGS	E	5600	-	-	X	-
4	AGS	F	6600	-	-	-	X
5	BCM	C	3701	-	-	-	X
5	BCM	D	4701	-	-	-	X
5	BCM	F	6701	-	-	X	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19802 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 RNA chain called 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	G	2	40	18	5	15	2	0	0	0
1	M	2	40	18	5	15	2	0	0	0
1	H	2	40	18	5	15	2	0	0	0
1	J	2	40	18	5	15	2	0	0	0
1	K	2	40	18	5	15	2	0	0	0
1	L	2	37	18	5	13	1	0	0	0

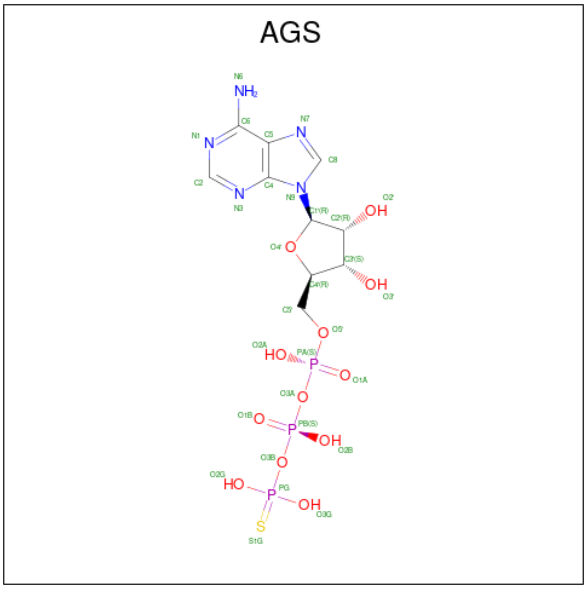
- Molecule 2 is a protein called Rho transcription termination factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	408	3210	2027	564	602	17	0	0	0
2	B	408	3213	2028	564	604	17	0	0	0
2	C	408	3213	2028	564	604	17	0	0	0
2	D	408	3213	2028	564	604	17	0	0	0
2	E	407	3206	2023	563	603	17	0	0	0
2	F	408	3213	2028	564	604	17	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0
3	F	1	1	1	0	0

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



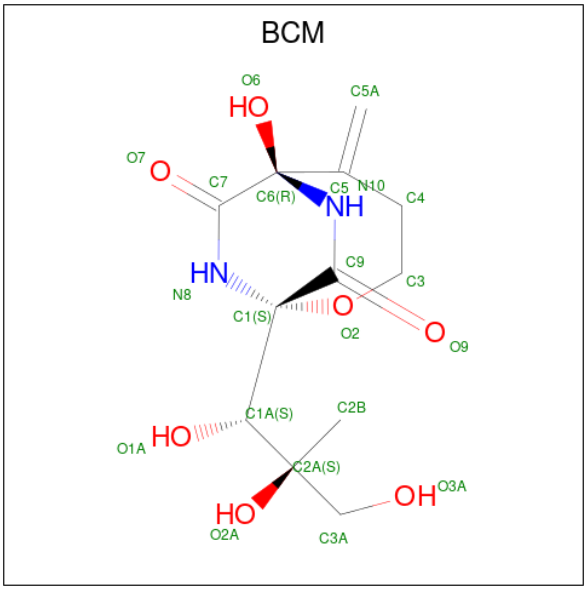
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	31	10	5	12	3	1	0	0
4	B	1	31	10	5	12	3	1	0	0
4	C	1	31	10	5	12	3	1	0	0
4	D	1	31	10	5	12	3	1	0	0
4	E	1	31	10	5	12	3	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	F	1	31	10	5	12	3	1	0	0

- Molecule 5 is BICYCLOMYCIN (three-letter code: BCM) (formula: $C_{12}H_{18}N_2O_7$).



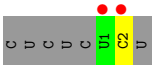
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	21	12	2	7	0	0
5	C	1	21	12	2	7	0	0
5	D	1	21	12	2	7	0	0
5	E	1	21	12	2	7	0	0
5	F	1	21	12	2	7	0	0

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.

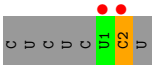
• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain G:



• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain M:

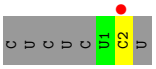


• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain H:

• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain J:

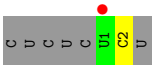


• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

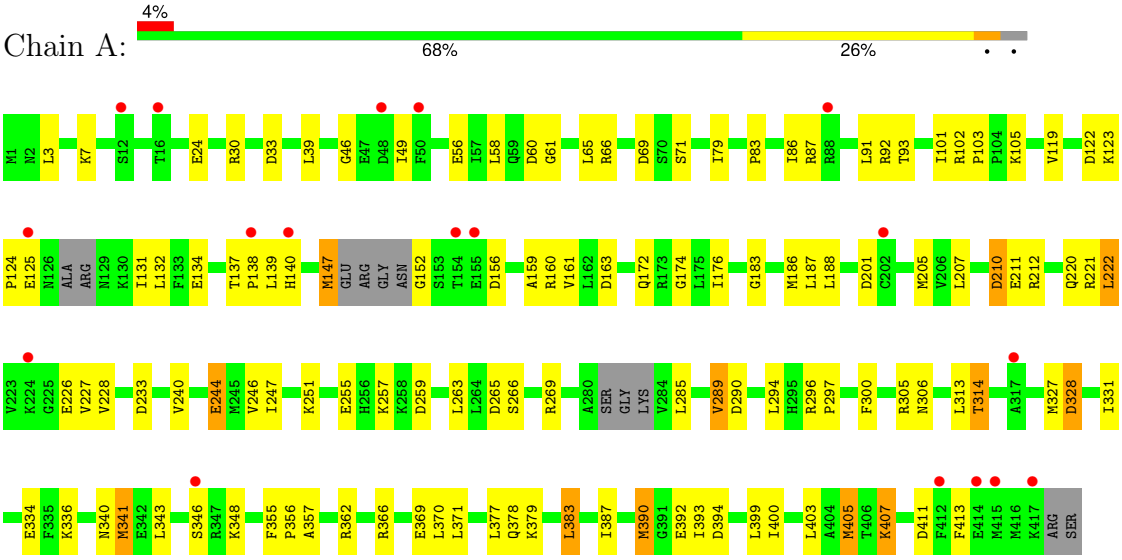
Chain K:

• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

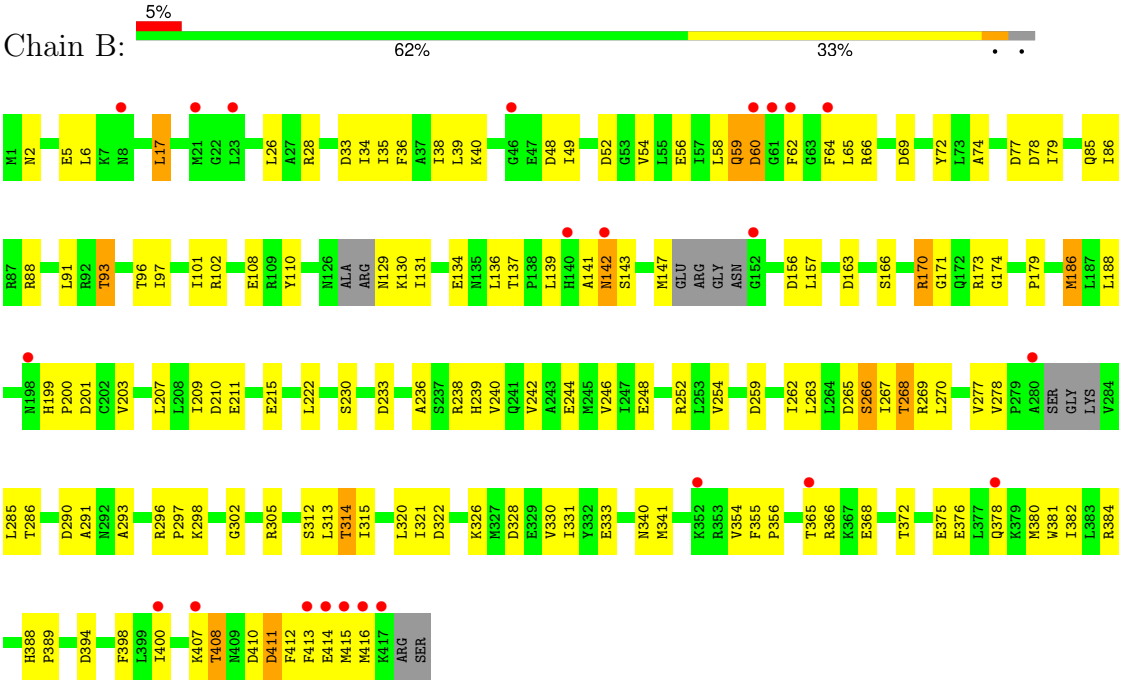
Chain L:



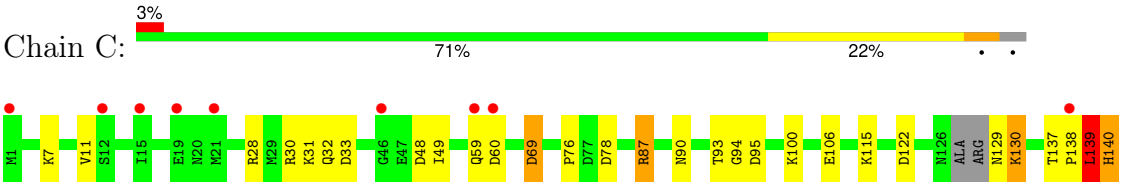
• Molecule 2: Rho transcription termination factor

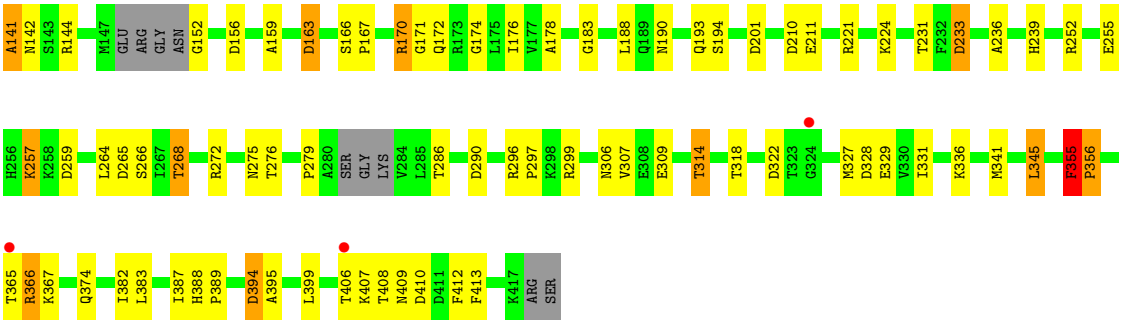


• Molecule 2: Rho transcription termination factor



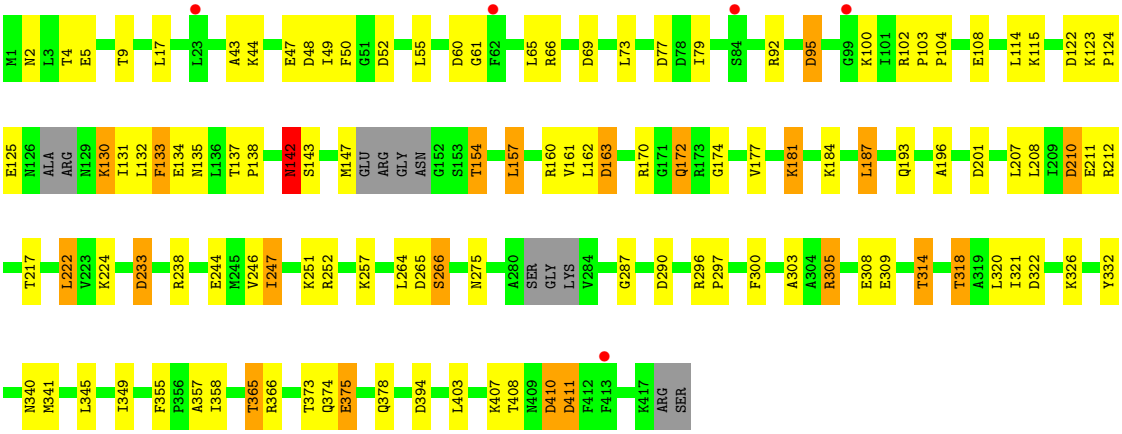
• Molecule 2: Rho transcription termination factor





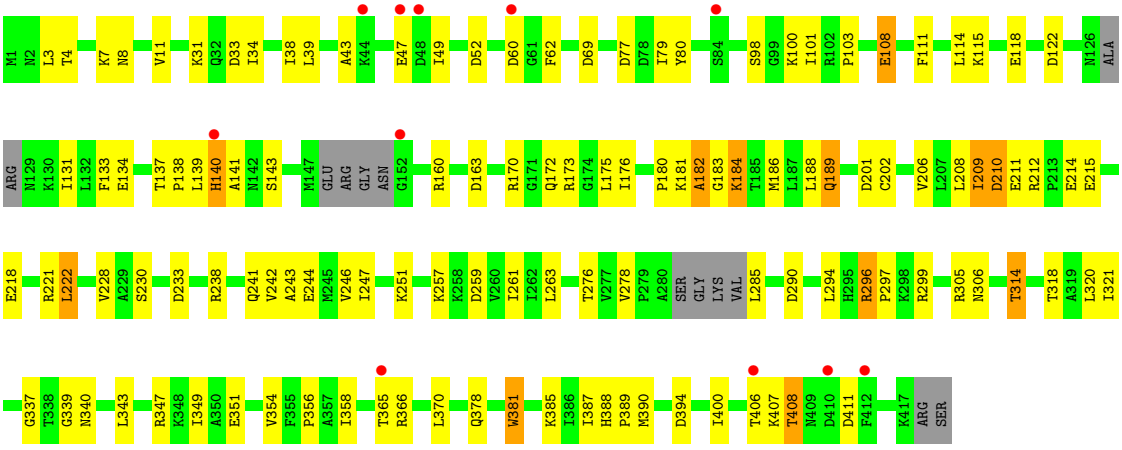
- Molecule 2: Rho transcription termination factor

Chain D:



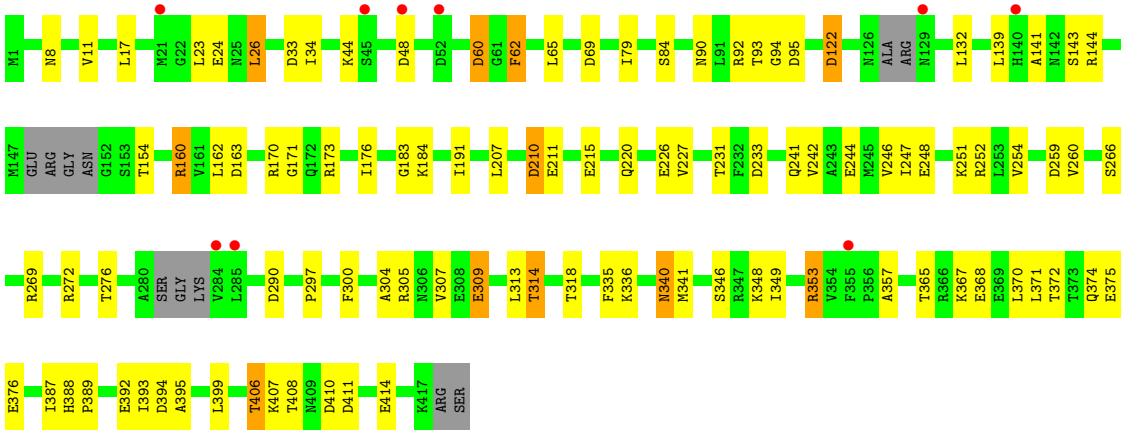
- Molecule 2: Rho transcription termination factor

Chain E:



- Molecule 2: Rho transcription termination factor

Chain F:


M1 N8 V11 L17 M21 G22 L23 E24 N25 L26 D33 I34 K44 S45 D48 D52 D60 G61 F62 L65 D69 I79 S84 N90 L91 R92 T93 G94 D95 D122 N126 ALA ARG N129 L132 L139 H140 A141 N142 S143 R144
M147 GLU ARG GLY ASN G152 S153 T154 R160 V161 L162 D163 R170 G171 Q172 R173 I176 G183 K184 I191 L207 D210 E211 E215 Q220 E226 V227 T231 F232 D233 Q241 V242 A243 E244 M245 V246 I247 E248 K251 R252 L253 V254 D259 V260 S266
R269 R272 T276 A280 SER GLY LYS V284 L285 D290 P297 F300 A304 R305 N306 V307 E308 E309 L313 T314 T318 F335 K336 M340 M341 S346 R347 K348 I349 R353 V354 F355 P356 A357 T365 R366 K367 E368 E369 L370 L371 T372 T373 Q374 E375
E376 I387 H388 P389 E392 I393 D394 A395 L399 T406 K407 T408 M409 D410 D411 E414 K417 ARG SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.93Å 111.37Å 161.03Å 90.00° 108.79° 90.00°	Depositor
Resolution (Å)	20.00 – 3.15 28.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.6 (20.00-3.15) 68.0 (28.95-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.285 , 0.306 0.276 , 0.294	Depositor DCC
R_{free} test set	2990 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	108.9	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 113.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19802	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: MG, AGS, BCM

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	G	0.79	0/43	1.10	0/64
1	H	0.76	0/43	0.90	0/64
1	J	0.72	0/43	1.08	0/64
1	K	0.66	0/43	0.93	0/64
1	L	0.77	0/40	1.24	0/60
1	M	0.69	0/43	1.28	0/64
2	A	0.30	0/3256	0.65	13/4383 (0.3%)
2	B	0.31	0/3259	0.65	15/4387 (0.3%)
2	C	0.30	0/3259	0.65	15/4387 (0.3%)
2	D	0.30	0/3259	0.66	15/4387 (0.3%)
2	E	0.30	0/3252	0.64	10/4377 (0.2%)
2	F	0.30	0/3259	0.64	14/4387 (0.3%)
All	All	0.31	0/19799	0.66	82/26688 (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	C	0	1

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	69	ASP	CB-CG-OD2	6.28	123.95	118.30
2	D	322	ASP	CB-CG-OD2	6.15	123.83	118.30
2	D	77	ASP	CB-CG-OD2	6.09	123.78	118.30
2	E	233	ASP	CB-CG-OD2	6.06	123.75	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	233	ASP	CB-CG-OD2	5.98	123.68	118.30
2	D	48	ASP	CB-CG-OD2	5.94	123.65	118.30
2	B	233	ASP	CB-CG-OD2	5.94	123.65	118.30
2	B	290	ASP	CB-CG-OD2	5.94	123.65	118.30
2	A	394	ASP	CB-CG-OD2	5.92	123.62	118.30
2	A	259	ASP	CB-CG-OD2	5.90	123.61	118.30
2	D	410	ASP	CB-CG-OD2	5.89	123.61	118.30
2	B	156	ASP	CB-CG-OD2	5.89	123.60	118.30
2	E	163	ASP	CB-CG-OD2	5.87	123.58	118.30
2	B	328	ASP	CB-CG-OD2	5.85	123.57	118.30
2	C	394	ASP	CB-CG-OD2	5.84	123.56	118.30
2	A	33	ASP	CB-CG-OD2	5.83	123.55	118.30
2	F	410	ASP	CB-CG-OD2	5.83	123.55	118.30
2	D	394	ASP	CB-CG-OD2	5.82	123.54	118.30
2	D	52	ASP	CB-CG-OD2	5.80	123.52	118.30
2	E	394	ASP	CB-CG-OD2	5.79	123.51	118.30
2	F	163	ASP	CB-CG-OD2	5.74	123.47	118.30
2	F	95	ASP	CB-CG-OD2	5.74	123.47	118.30
2	A	163	ASP	CB-CG-OD2	5.70	123.43	118.30
2	F	122	ASP	CB-CG-OD2	5.69	123.42	118.30
2	F	48	ASP	CB-CG-OD2	5.68	123.42	118.30
2	E	259	ASP	CB-CG-OD2	5.66	123.40	118.30
2	D	233	ASP	CB-CG-OD2	5.63	123.36	118.30
2	D	95	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	77	ASP	CB-CG-OD2	5.57	123.31	118.30
2	A	69	ASP	CB-CG-OD2	5.53	123.28	118.30
2	D	60	ASP	CB-CG-OD2	5.45	123.21	118.30
2	F	60	ASP	CB-CG-OD2	5.43	123.19	118.30
2	C	233	ASP	CB-CG-OD2	5.42	123.18	118.30
2	F	33	ASP	CB-CG-OD2	5.37	123.13	118.30
2	A	156	ASP	CB-CG-OD2	5.34	123.11	118.30
2	B	394	ASP	CB-CG-OD2	5.32	123.09	118.30
2	A	265	ASP	CB-CG-OD2	5.28	123.05	118.30
2	C	78	ASP	CB-CG-OD2	5.28	123.05	118.30
2	D	290	ASP	CB-CG-OD2	5.25	123.02	118.30
2	D	210	ASP	CB-CG-OD2	5.24	123.02	118.30
2	D	265	ASP	CB-CG-OD2	5.24	123.02	118.30
2	A	233	ASP	CB-CG-OD2	5.24	123.02	118.30
2	E	52	ASP	CB-CG-OD2	5.24	123.01	118.30
2	C	163	ASP	CB-CG-OD2	5.23	123.01	118.30
2	E	210	ASP	CB-CG-OD2	5.22	123.00	118.30
2	E	77	ASP	CB-CG-OD2	5.22	123.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	163	ASP	CB-CG-OD2	5.20	122.98	118.30
2	C	95	ASP	CB-CG-OD2	5.20	122.98	118.30
2	D	163	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	322	ASP	CB-CG-OD2	5.17	122.95	118.30
2	F	210	ASP	CB-CG-OD2	5.15	122.94	118.30
2	E	201	ASP	CB-CG-OD2	5.15	122.93	118.30
2	C	60	ASP	CB-CG-OD2	5.14	122.92	118.30
2	C	33	ASP	CB-CG-OD2	5.13	122.92	118.30
2	A	201	ASP	CB-CG-OD2	5.13	122.91	118.30
2	B	52	ASP	CB-CG-OD2	5.12	122.90	118.30
2	A	328	ASP	CB-CG-OD2	5.11	122.90	118.30
2	F	290	ASP	CB-CG-OD2	5.11	122.90	118.30
2	B	259	ASP	CB-CG-OD2	5.10	122.89	118.30
2	D	411	ASP	CB-CG-OD2	5.10	122.89	118.30
2	E	33	ASP	CB-CG-OD2	5.09	122.89	118.30
2	F	411	ASP	CB-CG-OD2	5.09	122.89	118.30
2	C	259	ASP	CB-CG-OD2	5.09	122.88	118.30
2	F	394	ASP	CB-CG-OD2	5.08	122.88	118.30
2	C	210	ASP	CB-CG-OD2	5.08	122.87	118.30
2	E	60	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	201	ASP	CB-CG-OD2	5.07	122.86	118.30
2	B	210	ASP	CB-CG-OD2	5.07	122.86	118.30
2	C	69	ASP	CB-CG-OD2	5.07	122.86	118.30
2	A	290	ASP	CB-CG-OD2	5.06	122.86	118.30
2	B	69	ASP	CB-CG-OD2	5.06	122.85	118.30
2	C	156	ASP	CB-CG-OD2	5.05	122.85	118.30
2	C	48	ASP	CB-CG-OD2	5.05	122.84	118.30
2	C	201	ASP	CB-CG-OD2	5.05	122.84	118.30
2	D	201	ASP	CB-CG-OD2	5.04	122.83	118.30
2	A	60	ASP	CB-CG-OD2	5.03	122.83	118.30
2	B	48	ASP	CB-CG-OD2	5.03	122.83	118.30
2	C	322	ASP	CB-CG-OD2	5.03	122.82	118.30
2	F	259	ASP	CB-CG-OD2	5.03	122.82	118.30
2	C	265	ASP	CB-CG-OD2	5.02	122.81	118.30
2	A	210	ASP	CB-CG-OD2	5.01	122.81	118.30
2	B	265	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	355	PHE	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	G	40	0	22	0	0
1	H	40	0	22	0	0
1	J	40	0	22	0	0
1	K	40	0	22	1	0
1	L	37	0	23	0	0
1	M	40	0	22	3	0
2	A	3210	0	3287	57	0
2	B	3213	0	3289	78	0
2	C	3213	0	3289	56	0
2	D	3213	0	3288	59	0
2	E	3206	0	3280	71	0
2	F	3213	0	3289	41	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	2	0
4	C	31	0	12	1	0
4	D	31	0	12	4	0
4	E	31	0	12	12	0
4	F	31	0	12	3	0
5	B	21	0	18	4	0
5	C	21	0	18	4	0
5	D	21	0	18	5	0
5	E	21	0	18	2	0
5	F	21	0	18	7	0
All	All	19802	0	20017	362	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 9.

All (362) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:ARG:NE	4:C:3600:AGS:S1G	2.30	1.05
2:D:366:ARG:NH2	4:E:5600:AGS:PG	2.33	1.02
2:D:366:ARG:NH1	4:E:5600:AGS:S1G	2.36	0.97
2:D:366:ARG:CZ	4:E:5600:AGS:S1G	2.53	0.96
2:A:140:HIS:CD2	2:A:340:ASN:HD22	1.83	0.95
2:E:183:GLY:O	2:E:184:LYS:HG2	1.70	0.91
2:A:140:HIS:CD2	2:A:340:ASN:ND2	2.39	0.90
2:C:355:PHE:HB3	2:C:356:PRO:CD	2.04	0.87
2:E:228:VAL:HG21	2:E:246:VAL:HG21	1.58	0.83
2:C:407:LYS:O	2:C:410:ASP:HB2	1.79	0.82
2:D:138:PRO:HG2	2:D:308:GLU:HB3	1.61	0.82
2:E:408:THR:O	2:E:411:ASP:CG	2.20	0.79
2:B:60:ASP:CB	2:B:62:PHE:CE2	2.66	0.78
2:C:355:PHE:HB3	2:C:356:PRO:HD2	1.66	0.78
2:C:355:PHE:CB	2:C:356:PRO:HD2	2.15	0.77
2:F:141:ALA:HB1	2:F:370:LEU:HB2	1.66	0.76
2:B:60:ASP:HB3	2:B:62:PHE:CE2	2.20	0.75
2:B:171:GLY:H	2:B:314:THR:HG22	1.51	0.74
2:A:140:HIS:CG	2:A:340:ASN:ND2	2.54	0.74
2:F:171:GLY:H	2:F:314:THR:HG23	1.54	0.72
2:B:413:PHE:CE1	2:B:414:GLU:HG3	2.25	0.72
2:D:73:LEU:HB2	2:D:238:ARG:HH21	1.56	0.71
2:B:137:THR:HG21	2:B:305:ARG:HD3	1.73	0.71
2:E:134:GLU:HB3	2:F:11:VAL:HG21	1.74	0.70
2:A:340:ASN:HA	2:A:366:ARG:HD2	1.74	0.70
2:D:366:ARG:CZ	4:E:5600:AGS:PG	2.79	0.70
2:A:289:VAL:HG13	2:A:327:MET:HG2	1.75	0.69
2:C:388:HIS:HB3	2:C:389:PRO:HD3	1.73	0.68
2:A:147:MET:HB3	2:A:159:ALA:HB1	1.76	0.67
2:D:187:LEU:HD12	2:D:345:LEU:HD11	1.75	0.67
2:A:139:LEU:O	2:A:306:ASN:HB3	1.95	0.67
2:E:186:MET:HG2	4:E:5600:AGS:C5	2.25	0.67
2:E:183:GLY:O	2:E:184:LYS:CG	2.42	0.67
2:C:387:ILE:HG23	2:C:395:ALA:HB1	1.77	0.67
2:D:143:SER:HB2	2:D:170:ARG:HD2	1.76	0.67
2:A:49:ILE:HD12	2:A:101:ILE:HG13	1.79	0.65
5:F:6701:BCM:HA1	5:F:6701:BCM:O9	1.97	0.64
2:A:3:LEU:HD13	2:A:39:LEU:HD11	1.78	0.63
2:D:65:LEU:HB2	2:D:79:ILE:HB	1.80	0.63
2:A:172:GLN:H	2:A:314:THR:HB	1.63	0.63
2:B:85:GLN:HA	2:B:88:ARG:HD3	1.80	0.63
2:C:341:MET:HG2	2:C:365:THR:HG22	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:247:ILE:O	2:E:251:LYS:HB2	1.98	0.63
2:F:307:VAL:HG13	2:F:309:GLU:HG2	1.81	0.63
2:A:131:ILE:HG13	2:A:134:GLU:HG2	1.79	0.63
2:B:6:LEU:HB3	2:B:35:ILE:HD12	1.79	0.62
2:A:355:PHE:N	2:A:356:PRO:HD2	2.14	0.62
2:D:177:VAL:HG13	2:D:321:ILE:HD13	1.82	0.62
2:A:186:MET:HB2	4:A:1600:AGS:O2A	2.00	0.61
2:C:174:GLY:HA2	2:C:341:MET:HB3	1.81	0.61
2:B:64:PHE:CD1	2:B:78:ASP:HB3	2.34	0.61
5:B:2701:BCM:HA1	5:B:2701:BCM:O9	1.99	0.61
2:E:337:GLY:O	5:F:6701:BCM:H32	2.01	0.61
2:B:230:SER:HB3	2:B:242:VAL:HG21	1.81	0.61
2:E:141:ALA:HB1	2:E:370:LEU:HB3	1.81	0.61
5:D:4701:BCM:C9	5:D:4701:BCM:HA2	2.30	0.61
2:E:180:PRO:HA	4:E:5600:AGS:O3G	2.01	0.60
2:E:366:ARG:NE	4:F:6600:AGS:S1G	2.70	0.60
2:E:100:LYS:HD3	2:E:114:LEU:HD23	1.84	0.60
2:F:23:LEU:HB3	2:F:26:LEU:HD21	1.84	0.60
2:D:355:PHE:CZ	4:D:4600:AGS:H1'	2.37	0.59
2:E:176:ILE:HB	2:E:318:THR:HG22	1.84	0.59
2:C:140:HIS:HB3	2:C:306:ASN:HB3	1.85	0.59
2:E:181:LYS:HG2	4:E:5600:AGS:S1G	2.42	0.59
2:B:355:PHE:N	2:B:356:PRO:HD2	2.17	0.59
2:C:172:GLN:H	2:C:314:THR:HB	1.67	0.59
2:A:140:HIS:CG	2:A:340:ASN:HD21	2.19	0.59
2:A:366:ARG:NE	4:B:2600:AGS:S1G	2.76	0.58
2:E:137:THR:HG22	2:E:305:ARG:HD3	1.86	0.58
2:A:65:LEU:HB2	2:A:79:ILE:HB	1.86	0.58
2:A:210:ASP:HB3	2:A:269:ARG:HD2	1.86	0.58
2:A:369:GLU:HA	2:A:377:LEU:HD11	1.85	0.58
2:A:86:ILE:HG23	2:A:91:LEU:HB2	1.84	0.58
2:B:240:VAL:HG21	2:B:277:VAL:HG11	1.86	0.58
2:D:43:ALA:HB1	2:D:103:PRO:HG3	1.86	0.57
2:A:379:LYS:O	2:A:383:LEU:HB2	2.03	0.57
2:F:254:VAL:HG21	2:F:313:LEU:HB2	1.85	0.57
2:A:174:GLY:HA2	2:A:341:MET:HB3	1.86	0.57
2:E:80:TYR:HB3	2:E:111:PHE:O	2.06	0.56
2:E:408:THR:O	2:E:411:ASP:OD2	2.23	0.56
2:C:140:HIS:CD2	2:C:306:ASN:H	2.22	0.56
2:E:172:GLN:H	2:E:314:THR:HB	1.69	0.56
2:B:268:THR:HG21	2:B:320:LEU:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:ARG:HD2	4:D:4600:AGS:S1G	2.46	0.56
2:B:296:ARG:HB2	2:B:297:PRO:HD3	1.88	0.55
2:E:138:PRO:HD2	2:E:306:ASN:O	2.06	0.55
2:E:140:HIS:HA	2:E:306:ASN:HB2	1.88	0.55
2:E:34:ILE:O	2:E:38:ILE:HG12	2.07	0.55
2:D:137:THR:O	2:E:214:GLU:HA	2.06	0.55
2:D:172:GLN:H	2:D:314:THR:HB	1.72	0.54
2:B:340:ASN:HA	2:B:366:ARG:HH11	1.72	0.54
5:E:5701:BCM:C7	5:E:5701:BCM:H32	2.38	0.54
2:A:56:GLU:HA	2:A:93:THR:HG23	1.88	0.54
2:B:86:ILE:HA	2:B:91:LEU:HD11	1.89	0.54
2:D:408:THR:O	2:D:411:ASP:HB2	2.07	0.54
2:F:266:SER:HB3	5:F:6701:BCM:O3A	2.08	0.54
2:E:98:SER:HB2	2:E:118:GLU:HB2	1.90	0.53
2:D:142:ASN:HD22	2:D:142:ASN:N	2.06	0.53
2:A:266:SER:HB3	2:A:269:ARG:HB2	1.90	0.53
5:C:3701:BCM:C7	5:C:3701:BCM:H32	2.34	0.53
2:D:132:LEU:HD13	2:D:251:LYS:HA	1.91	0.53
2:D:303:ALA:O	2:D:305:ARG:HD2	2.09	0.53
5:B:2701:BCM:C7	5:B:2701:BCM:H32	2.39	0.53
2:C:140:HIS:CG	2:C:306:ASN:H	2.26	0.53
2:B:65:LEU:HD21	2:B:97:ILE:HB	1.91	0.53
2:D:174:GLY:HA2	2:D:341:MET:HB3	1.91	0.53
2:C:211:GLU:HA	5:C:3701:BCM:HB2	1.91	0.52
2:E:181:LYS:CG	4:E:5600:AGS:S1G	2.97	0.52
5:C:3701:BCM:C7	5:C:3701:BCM:C3	2.87	0.52
2:E:184:LYS:HZ2	2:E:320:LEU:HD22	1.75	0.52
2:B:248:GLU:O	2:B:252:ARG:HG2	2.10	0.52
2:F:183:GLY:HA2	4:F:6600:AGS:H8	1.92	0.52
2:E:182:ALA:O	4:E:5600:AGS:H8	2.10	0.52
2:B:129:ASN:O	2:C:28:ARG:HG3	2.10	0.52
2:E:340:ASN:HA	2:E:366:ARG:HD2	1.92	0.52
2:F:340:ASN:N	2:F:340:ASN:HD22	2.08	0.51
2:D:130:LYS:HD3	2:D:135:ASN:HD21	1.76	0.51
2:D:196:ALA:HB1	2:D:224:LYS:HB3	1.91	0.51
1:K:1:U:H3	2:E:108:GLU:CD	2.13	0.51
2:B:2:ASN:HD22	2:B:5:GLU:HB2	1.76	0.51
2:B:54:VAL:HG22	2:B:96:THR:HG22	1.91	0.51
2:E:160:ARG:NH2	2:E:407:LYS:HG2	2.25	0.51
2:B:211:GLU:HA	5:B:2701:BCM:HB2	1.92	0.51
2:D:104:PRO:HB2	2:D:108:GLU:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:238:ARG:HG3	2:D:238:ARG:HH11	1.75	0.51
2:A:211:GLU:HG3	2:A:212:ARG:N	2.25	0.51
2:B:236:ALA:HA	2:B:239:HIS:HD2	1.76	0.51
2:D:366:ARG:NH2	2:E:212:ARG:HH22	2.09	0.51
2:B:388:HIS:HB3	2:B:389:PRO:HD3	1.93	0.51
2:D:341:MET:HG2	2:D:365:THR:HB	1.92	0.51
2:B:65:LEU:HB2	2:B:79:ILE:HB	1.93	0.50
2:C:193:GLN:HE22	2:C:224:LYS:HG2	1.77	0.50
2:E:209:ILE:HD11	2:E:243:ALA:HB2	1.92	0.50
2:A:188:LEU:HD22	2:A:263:LEU:HB3	1.92	0.50
2:B:170:ARG:HG2	2:B:312:SER:OG	2.10	0.50
2:C:406:THR:HB	2:C:410:ASP:CB	2.40	0.50
2:E:381:TRP:HA	2:E:381:TRP:CE3	2.46	0.50
2:B:35:ILE:HA	2:B:38:ILE:HG22	1.93	0.50
2:C:87:ARG:HH11	2:C:87:ARG:HB2	1.77	0.50
2:F:211:GLU:HA	5:F:6701:BCM:HB2	1.91	0.50
2:A:71:SER:HA	2:A:228:VAL:HG12	1.94	0.50
2:A:160:ARG:HD2	2:A:403:LEU:HG	1.92	0.50
2:B:60:ASP:HB2	2:B:62:PHE:CE2	2.47	0.50
2:E:181:LYS:H	4:E:5600:AGS:PG	2.35	0.50
2:B:267:ILE:HD12	2:B:270:LEU:HD23	1.94	0.49
2:D:296:ARG:N	2:D:297:PRO:HD2	2.27	0.49
2:C:355:PHE:O	2:C:356:PRO:C	2.50	0.49
5:E:5701:BCM:C7	5:E:5701:BCM:C3	2.89	0.49
2:A:152:GLY:HA2	2:A:160:ARG:HH22	1.78	0.49
2:B:372:THR:HB	2:B:376:GLU:HB3	1.94	0.49
2:C:138:PRO:C	2:C:140:HIS:H	2.14	0.49
2:D:47:GLU:HG3	2:D:100:LYS:HG2	1.95	0.49
2:F:160:ARG:HH21	2:F:407:LYS:HD3	1.78	0.49
2:E:347:ARG:O	2:E:351:GLU:HG2	2.13	0.49
2:B:136:LEU:HD13	2:C:221:ARG:HH22	1.77	0.49
2:B:174:GLY:HA2	2:B:341:MET:HB3	1.95	0.49
2:B:378:GLN:O	2:B:382:ILE:HG12	2.12	0.49
2:D:355:PHE:CE1	4:D:4600:AGS:C1'	2.96	0.49
2:C:299:ARG:HG2	2:D:233:ASP:HB3	1.95	0.49
2:E:388:HIS:HB3	2:E:389:PRO:HD3	1.94	0.49
2:D:102:ARG:HG2	2:D:114:LEU:HD13	1.95	0.49
2:E:11:VAL:HG22	2:E:31:LYS:HD2	1.94	0.49
5:B:2701:BCM:C7	5:B:2701:BCM:C3	2.90	0.49
2:F:346:SER:H	2:F:357:ALA:HB1	1.77	0.48
2:E:31:LYS:HA	2:E:34:ILE:HD12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:296:ARG:HB2	2:C:297:PRO:HD3	1.94	0.48
5:F:6701:BCM:C7	5:F:6701:BCM:C3	2.91	0.48
2:A:137:THR:HG23	2:A:305:ARG:HB2	1.94	0.48
2:B:408:THR:O	2:B:411:ASP:OD1	2.31	0.48
2:A:355:PHE:H	2:A:356:PRO:HD2	1.78	0.48
2:C:268:THR:O	2:C:272:ARG:HG2	2.13	0.48
2:D:366:ARG:NH2	4:E:5600:AGS:O3B	2.47	0.48
2:C:11:VAL:HG22	2:C:31:LYS:HD2	1.95	0.48
2:D:2:ASN:HB3	2:D:50:PHE:HB2	1.96	0.48
2:A:3:LEU:HG	2:A:7:LYS:HE2	1.95	0.48
2:D:133:PHE:H	2:D:133:PHE:HD1	1.62	0.47
2:F:62:PHE:H	2:F:62:PHE:HD2	1.61	0.47
2:A:370:LEU:HD23	2:A:370:LEU:H	1.79	0.47
2:B:66:ARG:HB2	2:B:72:TYR:HD1	1.79	0.47
2:B:59:GLN:O	2:B:60:ASP:CG	2.52	0.47
2:E:43:ALA:HB1	2:E:103:PRO:HG3	1.95	0.47
2:F:260:VAL:HB	2:F:313:LEU:HD12	1.96	0.47
2:D:266:SER:H	2:D:318:THR:HG23	1.80	0.47
5:F:6701:BCM:H32	5:F:6701:BCM:C7	2.42	0.47
2:B:354:VAL:HG13	2:B:400:ILE:HD12	1.97	0.47
2:C:152:GLY:HA3	2:C:407:LYS:HE2	1.97	0.47
2:E:208:LEU:HB3	2:E:211:GLU:HB2	1.97	0.47
2:F:139:LEU:HD22	2:F:367:LYS:HZ3	1.79	0.47
2:F:341:MET:HG2	2:F:365:THR:HG22	1.97	0.47
1:M:2:C:N4	2:B:66:ARG:HH12	2.11	0.47
2:A:240:VAL:O	2:A:244:GLU:HB2	2.15	0.47
2:F:65:LEU:HB2	2:F:79:ILE:HB	1.97	0.47
2:A:383:LEU:O	2:A:387:ILE:HG12	2.14	0.47
2:B:78:ASP:HB2	2:B:110:TYR:CD1	2.50	0.47
2:C:306:ASN:CG	2:C:306:ASN:O	2.53	0.47
2:E:4:THR:HA	2:E:7:LYS:HD3	1.97	0.46
2:F:348:LYS:HB3	2:F:393:ILE:HD11	1.96	0.46
2:B:26:LEU:HD13	2:B:34:ILE:HG23	1.96	0.46
2:C:137:THR:HA	2:C:140:HIS:NE2	2.30	0.46
2:E:181:LYS:N	4:E:5600:AGS:O3G	2.38	0.46
2:E:343:LEU:HD21	2:E:358:ILE:HG12	1.96	0.46
2:F:143:SER:OG	2:F:170:ARG:HB2	2.15	0.46
2:F:220:GLN:HA	2:F:227:VAL:HG21	1.96	0.46
2:F:368:GLU:HA	2:F:371:LEU:HD12	1.97	0.46
2:A:355:PHE:C	2:A:357:ALA:H	2.19	0.46
2:F:184:LYS:HD2	2:F:318:THR:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:392:GLU:HG3	2:A:393:ILE:H	1.81	0.46
2:B:209:ILE:HG12	2:B:270:LEU:HD13	1.97	0.46
2:A:328:ASP:HA	2:A:331:ILE:HD12	1.98	0.46
2:C:366:ARG:HH12	5:D:4701:BCM:H42	1.81	0.46
2:E:100:LYS:HG3	2:E:115:LYS:H	1.80	0.46
2:C:141:ALA:O	2:C:142:ASN:HB2	2.16	0.46
2:D:366:ARG:NH2	2:E:212:ARG:NH2	2.63	0.46
2:B:398:PHE:HZ	2:B:415:MET:SD	2.38	0.46
2:D:247:ILE:HD12	2:D:251:LYS:HE3	1.97	0.46
2:F:247:ILE:HB	2:F:300:PHE:CE1	2.50	0.46
2:F:349:ILE:HD11	2:F:392:GLU:HB2	1.97	0.46
2:C:406:THR:HB	2:C:410:ASP:HB3	1.97	0.46
2:F:162:LEU:HD13	2:F:191:ILE:HD11	1.98	0.46
2:F:248:GLU:O	2:F:252:ARG:HG2	2.16	0.46
2:B:291:ALA:HB1	2:C:276:THR:HB	1.97	0.46
2:C:355:PHE:HB2	2:C:356:PRO:HD2	1.94	0.46
2:C:366:ARG:NH1	2:D:181:LYS:HD2	2.31	0.45
2:C:171:GLY:HA3	2:C:306:ASN:HB2	1.99	0.45
2:D:157:LEU:O	2:D:161:VAL:HG23	2.16	0.45
5:D:4701:BCM:C7	5:D:4701:BCM:H32	2.44	0.45
2:B:134:GLU:OE1	2:C:30:ARG:HA	2.15	0.45
2:D:55:LEU:HD23	2:D:92:ARG:O	2.16	0.45
2:E:131:ILE:HG12	2:E:133:PHE:H	1.81	0.45
2:C:7:LYS:HD2	2:C:69:ASP:HB3	1.98	0.45
2:C:137:THR:O	2:D:217:THR:OG1	2.32	0.45
2:D:123:LYS:C	2:D:125:GLU:H	2.20	0.45
2:B:59:GLN:O	2:B:60:ASP:OD1	2.34	0.45
2:C:140:HIS:HA	2:C:306:ASN:HD22	1.82	0.45
2:D:373:THR:O	2:D:375:GLU:N	2.50	0.45
1:M:2:C:H42	2:B:74:ALA:HB1	1.82	0.45
2:B:143:SER:HB2	2:B:170:ARG:NE	2.32	0.45
2:B:254:VAL:HG21	2:B:313:LEU:HB2	1.97	0.45
2:D:321:ILE:HD11	2:D:332:TYR:CD1	2.52	0.45
2:F:388:HIS:HB3	2:F:389:PRO:HD3	1.99	0.45
2:B:380:MET:O	2:B:384:ARG:HG3	2.17	0.45
2:D:172:GLN:HG2	2:D:340:ASN:OD1	2.17	0.45
2:A:176:ILE:HG12	2:A:343:LEU:HB3	1.98	0.45
2:B:17:LEU:HB3	2:B:38:ILE:HD11	1.98	0.45
2:B:238:ARG:O	2:B:242:VAL:HG23	2.17	0.45
2:D:357:ALA:O	2:D:358:ILE:C	2.55	0.45
5:C:3701:BCM:HA1	5:C:3701:BCM:O9	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:LEU:HD21	5:D:4701:BCM:O3A	2.17	0.44
2:E:3:LEU:HG	2:E:7:LYS:HD2	2.00	0.44
2:A:132:LEU:HG	2:A:251:LYS:HG2	2.00	0.44
2:B:262:ILE:HB	2:B:315:ILE:HG12	2.00	0.44
2:D:207:LEU:HD13	2:D:246:VAL:HG21	2.00	0.44
2:E:261:ILE:HG12	2:E:314:THR:HG23	1.99	0.44
2:F:173:ARG:HG2	2:F:304:ALA:HB3	1.98	0.44
2:A:346:SER:HB3	2:A:348:LYS:HG2	1.99	0.44
2:F:183:GLY:CA	4:F:6600:AGS:H8	2.47	0.44
2:A:205:MET:HG2	2:A:226:GLU:HB3	2.00	0.44
2:A:220:GLN:HA	2:A:227:VAL:HG21	1.99	0.44
2:D:43:ALA:HB1	2:D:103:PRO:CG	2.48	0.44
2:E:206:VAL:HG22	2:E:263:LEU:HB2	1.99	0.44
2:A:131:ILE:HA	2:A:255:GLU:HG2	1.99	0.44
2:D:133:PHE:N	2:D:133:PHE:CD1	2.85	0.44
2:E:173:ARG:HB3	2:E:339:GLY:HA2	1.98	0.44
2:B:141:ALA:O	2:B:142:ASN:C	2.56	0.44
2:C:32:GLN:HB3	2:C:76:PRO:HD2	2.00	0.44
2:C:139:LEU:HD11	2:C:367:LYS:HE3	2.00	0.44
2:A:296:ARG:N	2:A:297:PRO:HD2	2.33	0.44
2:F:272:ARG:O	2:F:276:THR:HG22	2.18	0.44
2:A:407:LYS:H	2:A:407:LYS:HD2	1.82	0.43
2:B:58:LEU:O	2:B:60:ASP:N	2.51	0.43
2:D:147:MET:HG3	2:D:162:LEU:HD22	2.00	0.43
1:M:2:C:H42	2:B:66:ARG:HH12	1.67	0.43
2:C:138:PRO:O	2:C:140:HIS:N	2.51	0.43
2:C:140:HIS:CB	2:C:306:ASN:HB3	2.46	0.43
2:B:365:THR:HG23	2:B:368:GLU:HB3	2.00	0.43
2:C:176:ILE:HB	2:C:318:THR:HG22	2.01	0.43
2:E:4:THR:HG22	2:E:7:LYS:HZ2	1.84	0.43
2:E:79:ILE:HG12	2:E:101:ILE:HG12	2.01	0.43
2:A:123:LYS:O	2:A:125:GLU:N	2.51	0.43
2:D:132:LEU:HD22	2:D:251:LYS:HG2	2.00	0.43
2:A:207:LEU:HD13	2:A:246:VAL:HG21	2.00	0.43
2:E:218:GLU:O	2:E:222:LEU:HB2	2.19	0.43
2:E:349:ILE:HG22	2:E:354:VAL:HB	2.00	0.43
2:F:297:PRO:HB2	2:F:335:PHE:HZ	1.83	0.43
2:A:387:ILE:HG13	2:A:399:LEU:HD11	2.01	0.43
2:B:199:HIS:N	2:B:200:PRO:HD3	2.34	0.43
2:B:326:LYS:O	2:B:330:VAL:HG23	2.18	0.43
5:D:4701:BCM:C7	5:D:4701:BCM:C3	2.93	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:LYS:O	2:B:408:THR:HB	2.19	0.43
2:C:408:THR:O	2:C:409:ASN:HB3	2.18	0.43
2:E:184:LYS:NZ	2:E:320:LEU:HD22	2.34	0.43
2:D:355:PHE:CE1	4:D:4600:AGS:H1'	2.54	0.42
2:E:408:THR:O	2:E:411:ASP:OD1	2.37	0.42
2:F:387:ILE:HG23	2:F:395:ALA:HB1	2.01	0.42
2:B:412:PHE:CD1	2:B:413:PHE:N	2.87	0.42
2:C:406:THR:HB	2:C:410:ASP:HB2	2.00	0.42
2:E:184:LYS:O	2:E:188:LEU:HD12	2.19	0.42
2:F:26:LEU:HD12	2:F:34:ILE:HG12	2.02	0.42
2:F:132:LEU:HD22	2:F:251:LYS:HE2	2.01	0.42
2:D:366:ARG:CZ	2:E:212:ARG:NH2	2.82	0.42
2:E:172:GLN:N	2:E:314:THR:HB	2.35	0.42
2:A:92:ARG:HD3	2:B:28:ARG:HD3	2.02	0.42
2:E:356:PRO:HG2	2:E:400:ILE:HD11	2.00	0.42
2:C:257:LYS:HD3	2:C:309:GLU:O	2.20	0.42
2:F:207:LEU:HD13	2:F:246:VAL:HG21	2.00	0.42
2:C:327:MET:C	2:C:329:GLU:H	2.22	0.42
2:F:372:THR:HB	2:F:376:GLU:HB3	2.01	0.42
2:C:159:ALA:HB2	2:C:190:ASN:HD21	1.84	0.42
2:E:101:ILE:CG2	2:E:111:PHE:HB3	2.50	0.42
2:E:230:SER:HB2	2:E:242:VAL:HG11	2.02	0.42
2:B:36:PHE:O	2:B:40:LYS:HB2	2.20	0.42
2:D:208:LEU:HB3	2:D:211:GLU:HB2	2.01	0.42
2:B:173:ARG:HD3	2:B:302:GLY:HA2	2.01	0.41
2:B:207:LEU:HD13	2:B:246:VAL:HG21	2.02	0.41
2:E:189:GLN:HG2	2:E:222:LEU:HD12	2.02	0.41
2:A:403:LEU:HA	2:A:411:ASP:OD2	2.20	0.41
2:B:186:MET:HB3	4:B:2600:AGS:N7	2.35	0.41
2:B:179:PRO:HA	2:B:321:ILE:O	2.20	0.41
2:D:131:ILE:O	2:D:134:GLU:HG2	2.19	0.41
2:E:183:GLY:O	2:E:184:LYS:CB	2.67	0.41
2:A:119:VAL:N	2:A:122:ASP:O	2.54	0.41
2:A:160:ARG:HB3	2:A:403:LEU:HD21	2.02	0.41
2:B:188:LEU:HD12	2:B:263:LEU:HB3	2.01	0.41
2:F:406:THR:HB	2:F:407:LYS:H	1.53	0.41
2:B:60:ASP:HB3	2:B:62:PHE:CD2	2.54	0.41
2:B:166:SER:HB2	2:B:365:THR:HB	2.03	0.41
2:C:166:SER:HA	2:C:167:PRO:HD2	1.95	0.41
2:D:349:ILE:HD12	2:D:357:ALA:O	2.21	0.41
2:E:294:LEU:C	2:E:297:PRO:HD2	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:83:PRO:O	2:A:87:ARG:HG3	2.21	0.41
2:B:137:THR:CG2	2:B:305:ARG:HD3	2.43	0.41
2:B:266:SER:HB2	2:B:269:ARG:HB2	2.02	0.41
2:B:412:PHE:O	2:B:416:MET:HG2	2.21	0.41
2:D:366:ARG:CZ	2:E:212:ARG:HH22	2.33	0.41
2:B:277:VAL:HG13	2:B:278:VAL:HG23	2.02	0.41
2:B:356:PRO:CD	2:B:400:ILE:HD11	2.51	0.41
2:C:100:LYS:HB2	2:C:115:LYS:HB2	2.02	0.41
2:E:160:ARG:NH1	2:E:406:THR:O	2.54	0.41
2:E:385:LYS:HD2	2:F:353:ARG:NH2	2.36	0.41
2:A:102:ARG:HA	2:A:103:PRO:HD3	1.97	0.41
2:A:160:ARG:HD3	2:A:407:LYS:O	2.21	0.41
2:B:56:GLU:HA	2:B:93:THR:HB	2.03	0.41
2:C:268:THR:HA	2:C:331:ILE:HG21	2.02	0.41
2:E:62:PHE:HB2	2:E:80:TYR:HE1	1.86	0.41
2:E:296:ARG:N	2:E:297:PRO:CD	2.84	0.41
2:E:387:ILE:HG12	2:E:390:MET:HE3	2.03	0.41
2:F:176:ILE:HB	2:F:318:THR:HG22	2.03	0.41
2:A:183:GLY:O	2:A:187:LEU:HB2	2.21	0.41
2:A:294:LEU:HD13	2:A:334:GLU:HG3	2.03	0.41
2:B:326:LYS:H	2:B:326:LYS:HD3	1.86	0.40
2:C:275:ASN:HD21	2:C:290:ASP:H	1.69	0.40
2:D:123:LYS:O	2:D:125:GLU:N	2.44	0.40
2:F:244:GLU:O	2:F:248:GLU:HG2	2.21	0.40
2:C:130:LYS:O	2:C:255:GLU:HG2	2.20	0.40
2:C:178:ALA:HB2	2:C:345:LEU:HB2	2.04	0.40
2:D:264:LEU:HD22	2:D:300:PHE:CE2	2.56	0.40
2:F:266:SER:HB2	2:F:269:ARG:HB2	2.03	0.40
2:B:209:ILE:HG21	2:B:270:LEU:HB2	2.04	0.40
2:B:356:PRO:HD2	2:B:400:ILE:HD11	2.03	0.40
2:C:236:ALA:HA	2:C:239:HIS:HD2	1.86	0.40
2:E:170:ARG:NH1	2:E:202:CYS:SG	2.94	0.40
5:F:6701:BCM:C9	5:F:6701:BCM:C4	2.99	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
2	A	400/419 (96%)	328 (82%)	60 (15%)	12 (3%)	4 24
2	B	400/419 (96%)	356 (89%)	37 (9%)	7 (2%)	8 37
2	C	400/419 (96%)	357 (89%)	31 (8%)	12 (3%)	4 24
2	D	400/419 (96%)	343 (86%)	47 (12%)	10 (2%)	5 29
2	E	399/419 (95%)	361 (90%)	32 (8%)	6 (2%)	10 41
2	F	400/419 (96%)	360 (90%)	37 (9%)	3 (1%)	19 55
All	All	2399/2514 (95%)	2105 (88%)	244 (10%)	50 (2%)	7 33

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	407	LYS
2	B	142	ASN
2	B	408	THR
2	C	140	HIS
2	C	355	PHE
2	C	356	PRO
2	D	142	ASN
2	D	154	THR
2	D	184	LYS
2	D	374	GLN
2	E	143	SER
2	A	46	GLY
2	A	58	LEU
2	A	405	MET
2	B	60	ASP
2	B	293	ALA
2	C	139	LEU
2	C	141	ALA
2	C	279	PRO
2	C	307	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	408	THR
2	A	24	GLU
2	A	105	LYS
2	A	336	LYS
2	A	390	MET
2	B	266	SER
2	C	106	GLU
2	C	183	GLY
2	C	266	SER
2	E	140	HIS
2	F	44	LYS
2	A	124	PRO
2	A	222	LEU
2	B	59	GLN
2	C	170	ARG
2	D	44	LYS
2	D	287	GLY
2	E	49	ILE
2	E	182	ALA
2	F	24	GLU
2	B	410	ASP
2	C	94	GLY
2	D	266	SER
2	E	184	LYS
2	F	94	GLY
2	D	222	LEU
2	D	61	GLY
2	D	124	PRO
2	A	138	PRO
2	A	61	GLY

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
2	A	350/359 (98%)	327 (93%)	23 (7%)	16 47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	351/359 (98%)	322 (92%)	29 (8%)	11	37
2	C	351/359 (98%)	318 (91%)	33 (9%)	8	30
2	D	351/359 (98%)	311 (89%)	40 (11%)	5	23
2	E	350/359 (98%)	321 (92%)	29 (8%)	11	37
2	F	351/359 (98%)	320 (91%)	31 (9%)	10	34
All	All	2104/2154 (98%)	1919 (91%)	185 (9%)	10	34

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	30	ARG
2	A	66	ARG
2	A	147	MET
2	A	161	VAL
2	A	221	ARG
2	A	222	LEU
2	A	244	GLU
2	A	247	ILE
2	A	257	LYS
2	A	285	LEU
2	A	289	VAL
2	A	300	PHE
2	A	313	LEU
2	A	314	THR
2	A	341	MET
2	A	362	ARG
2	A	371	LEU
2	A	378	GLN
2	A	383	LEU
2	A	390	MET
2	A	400	ILE
2	A	405	MET
2	A	413	PHE
2	B	17	LEU
2	B	33	ASP
2	B	39	LEU
2	B	49	ILE
2	B	93	THR
2	B	101	ILE
2	B	102	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	108	GLU
2	B	130	LYS
2	B	131	ILE
2	B	139	LEU
2	B	147	MET
2	B	157	LEU
2	B	170	ARG
2	B	186	MET
2	B	203	VAL
2	B	215	GLU
2	B	222	LEU
2	B	244	GLU
2	B	268	THR
2	B	285	LEU
2	B	286	THR
2	B	298	LYS
2	B	314	THR
2	B	331	ILE
2	B	333	GLU
2	B	375	GLU
2	B	381	TRP
2	B	411	ASP
2	C	49	ILE
2	C	59	GLN
2	C	87	ARG
2	C	90	ASN
2	C	93	THR
2	C	122	ASP
2	C	129	ASN
2	C	130	LYS
2	C	139	LEU
2	C	144	ARG
2	C	163	ASP
2	C	170	ARG
2	C	188	LEU
2	C	194	SER
2	C	231	THR
2	C	233	ASP
2	C	252	ARG
2	C	257	LYS
2	C	264	LEU
2	C	268	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	286	THR
2	C	314	THR
2	C	328	ASP
2	C	336	LYS
2	C	345	LEU
2	C	366	ARG
2	C	374	GLN
2	C	382	ILE
2	C	383	LEU
2	C	394	ASP
2	C	399	LEU
2	C	412	PHE
2	C	413	PHE
2	D	4	THR
2	D	5	GLU
2	D	9	THR
2	D	17	LEU
2	D	49	ILE
2	D	66	ARG
2	D	69	ASP
2	D	95	ASP
2	D	115	LYS
2	D	122	ASP
2	D	130	LYS
2	D	133	PHE
2	D	142	ASN
2	D	154	THR
2	D	157	LEU
2	D	160	ARG
2	D	163	ASP
2	D	172	GLN
2	D	181	LYS
2	D	187	LEU
2	D	193	GLN
2	D	210	ASP
2	D	212	ARG
2	D	222	LEU
2	D	244	GLU
2	D	247	ILE
2	D	252	ARG
2	D	257	LYS
2	D	275	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	305	ARG
2	D	309	GLU
2	D	314	THR
2	D	318	THR
2	D	326	LYS
2	D	365	THR
2	D	375	GLU
2	D	378	GLN
2	D	403	LEU
2	D	407	LYS
2	D	410	ASP
2	E	8	ASN
2	E	39	LEU
2	E	47	GLU
2	E	69	ASP
2	E	108	GLU
2	E	122	ASP
2	E	139	LEU
2	E	175	LEU
2	E	189	GLN
2	E	209	ILE
2	E	210	ASP
2	E	215	GLU
2	E	221	ARG
2	E	222	LEU
2	E	238	ARG
2	E	241	GLN
2	E	244	GLU
2	E	257	LYS
2	E	276	THR
2	E	278	VAL
2	E	285	LEU
2	E	290	ASP
2	E	296	ARG
2	E	299	ARG
2	E	314	THR
2	E	321	ILE
2	E	365	THR
2	E	378	GLN
2	E	381	TRP
2	F	8	ASN
2	F	17	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	26	LEU
2	F	60	ASP
2	F	62	PHE
2	F	84	SER
2	F	90	ASN
2	F	92	ARG
2	F	93	THR
2	F	122	ASP
2	F	144	ARG
2	F	154	THR
2	F	160	ARG
2	F	210	ASP
2	F	215	GLU
2	F	226	GLU
2	F	231	THR
2	F	241	GLN
2	F	242	VAL
2	F	305	ARG
2	F	309	GLU
2	F	314	THR
2	F	336	LYS
2	F	340	ASN
2	F	353	ARG
2	F	374	GLN
2	F	375	GLU
2	F	399	LEU
2	F	406	THR
2	F	408	THR
2	F	414	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	32	GLN
2	A	140	HIS
2	A	275	ASN
2	A	292	ASN
2	A	340	ASN
2	B	2	ASN
2	B	126	ASN
2	B	129	ASN
2	B	142	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	193	GLN
2	B	275	ASN
2	B	292	ASN
2	C	20	ASN
2	C	25	ASN
2	C	90	ASN
2	C	117	ASN
2	C	190	ASN
2	C	193	GLN
2	C	198	ASN
2	C	220	GLN
2	C	275	ASN
2	C	306	ASN
2	C	388	HIS
2	D	20	ASN
2	D	135	ASN
2	D	140	HIS
2	D	142	ASN
2	D	306	ASN
2	D	361	ASN
2	D	374	GLN
2	D	401	ASN
2	E	8	ASN
2	E	241	GLN
2	E	374	GLN
2	F	8	ASN
2	F	90	ASN
2	F	135	ASN
2	F	256	HIS
2	F	306	ASN
2	F	340	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	1/8 (12%)	1 (100%)	0
1	H	1/8 (12%)	1 (100%)	0
1	J	1/8 (12%)	1 (100%)	0
1	K	1/8 (12%)	0	0
1	L	1/8 (12%)	1 (100%)	0
1	M	1/8 (12%)	1 (100%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	6/48 (12%)	5 (83%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	2	C
1	M	2	C
1	H	2	C
1	J	2	C
1	L	2	C

There are no RNA pucker outliers to report.

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)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

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	$\#\|Z\| > 2$
5	BCM	B	2701	3	14,22,22	1.16	1 (7%)	11,36,36	2.08	1 (9%)
5	BCM	D	4701	-	14,22,22	1.17	1 (7%)	11,36,36	2.09	2 (18%)
4	AGS	C	3600	3	28,33,33	2.23	7 (25%)	31,52,52	1.49	5 (16%)
4	AGS	B	2600	3	28,33,33	2.28	7 (25%)	31,52,52	1.49	4 (12%)
4	AGS	F	6600	3	28,33,33	2.28	7 (25%)	31,52,52	1.48	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AGS	A	1600	3	28,33,33	2.33	7 (25%)	31,52,52	1.48	4 (12%)
5	BCM	C	3701	3	14,22,22	1.14	1 (7%)	11,36,36	2.02	1 (9%)
5	BCM	F	6701	-	14,22,22	1.16	1 (7%)	11,36,36	2.00	1 (9%)
4	AGS	E	5600	3,2	28,33,33	2.41	7 (25%)	31,52,52	1.53	4 (12%)
5	BCM	E	5701	3	14,22,22	1.12	1 (7%)	11,36,36	2.11	2 (18%)
4	AGS	D	4600	3	28,33,33	2.33	6 (21%)	31,52,52	1.48	4 (12%)

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
5	BCM	B	2701	3	-	6/10/50/50	0/1/2/2
5	BCM	D	4701	-	-	4/10/50/50	0/1/2/2
4	AGS	C	3600	3	-	4/17/38/38	0/3/3/3
4	AGS	B	2600	3	-	2/17/38/38	0/3/3/3
4	AGS	F	6600	3	-	5/17/38/38	0/3/3/3
4	AGS	A	1600	3	-	3/17/38/38	0/3/3/3
5	BCM	C	3701	3	-	4/10/50/50	0/1/2/2
5	BCM	F	6701	-	-	6/10/50/50	0/1/2/2
4	AGS	E	5600	3,2	-	5/17/38/38	0/3/3/3
5	BCM	E	5701	3	-	7/10/50/50	0/1/2/2
4	AGS	D	4600	3	-	7/17/38/38	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5600	AGS	PG-S1G	8.30	2.08	1.90
4	A	1600	AGS	PG-S1G	7.63	2.07	1.90
4	D	4600	AGS	PG-S1G	7.63	2.07	1.90
4	B	2600	AGS	PG-S1G	7.30	2.06	1.90
4	F	6600	AGS	PG-S1G	7.23	2.06	1.90
4	C	3600	AGS	PG-S1G	7.04	2.05	1.90
4	D	4600	AGS	C4-N3	6.68	1.44	1.35
4	B	2600	AGS	C4-N3	6.66	1.44	1.35
4	A	1600	AGS	C4-N3	6.63	1.44	1.35
4	F	6600	AGS	C4-N3	6.59	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5600	AGS	C4-N3	6.58	1.44	1.35
4	C	3600	AGS	C4-N3	6.52	1.44	1.35
5	D	4701	BCM	O6-C6	3.65	1.44	1.40
5	F	6701	BCM	O6-C6	3.63	1.44	1.40
5	B	2701	BCM	O6-C6	3.57	1.44	1.40
5	C	3701	BCM	O6-C6	3.51	1.44	1.40
5	E	5701	BCM	O6-C6	3.49	1.43	1.40
4	F	6600	AGS	PA-O1A	2.61	1.59	1.50
4	E	5600	AGS	PA-O1A	2.61	1.59	1.50
4	D	4600	AGS	PA-O1A	2.60	1.59	1.50
4	C	3600	AGS	PA-O1A	2.59	1.59	1.50
4	A	1600	AGS	PA-O1A	2.59	1.59	1.50
4	B	2600	AGS	PA-O1A	2.58	1.59	1.50
4	D	4600	AGS	PB-O1B	2.51	1.59	1.50
4	F	6600	AGS	PB-O1B	2.50	1.59	1.50
4	B	2600	AGS	PB-O1B	2.49	1.59	1.50
4	E	5600	AGS	PB-O1B	2.46	1.59	1.50
4	A	1600	AGS	PB-O3A	2.46	1.62	1.59
4	C	3600	AGS	PB-O1B	2.42	1.59	1.50
4	A	1600	AGS	PB-O1B	2.38	1.59	1.50
4	F	6600	AGS	PB-O3A	2.37	1.62	1.59
4	E	5600	AGS	PB-O3A	2.37	1.62	1.59
4	C	3600	AGS	PA-O3A	2.31	1.62	1.59
4	C	3600	AGS	PB-O3A	2.31	1.62	1.59
4	A	1600	AGS	PA-O3A	2.30	1.62	1.59
4	D	4600	AGS	O4'-C1'	2.27	1.43	1.40
4	E	5600	AGS	PA-O3A	2.26	1.61	1.59
4	E	5600	AGS	O4'-C1'	2.25	1.43	1.40
4	F	6600	AGS	PA-O3A	2.19	1.61	1.59
4	B	2600	AGS	PB-O3A	2.18	1.61	1.59
4	C	3600	AGS	O4'-C1'	2.18	1.43	1.40
4	F	6600	AGS	O4'-C1'	2.13	1.43	1.40
4	B	2600	AGS	O4'-C1'	2.11	1.43	1.40
4	D	4600	AGS	PB-O3A	2.10	1.61	1.59
4	B	2600	AGS	PA-O3A	2.07	1.61	1.59
4	A	1600	AGS	PB-O3B	2.03	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2701	BCM	C7-C6-N10	6.12	117.69	109.66
5	E	5701	BCM	C7-C6-N10	6.12	117.69	109.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	4701	BCM	C7-C6-N10	6.02	117.56	109.66
5	F	6701	BCM	C7-C6-N10	5.95	117.46	109.66
5	C	3701	BCM	C7-C6-N10	5.91	117.41	109.66
4	A	1600	AGS	N3-C2-N1	-4.41	122.69	128.67
4	D	4600	AGS	N3-C2-N1	-4.32	122.80	128.67
4	E	5600	AGS	N3-C2-N1	-4.31	122.82	128.67
4	F	6600	AGS	N3-C2-N1	-4.29	122.86	128.67
4	B	2600	AGS	N3-C2-N1	-4.27	122.87	128.67
4	C	3600	AGS	N3-C2-N1	-4.26	122.90	128.67
4	E	5600	AGS	PB-O3B-PG	-3.69	119.65	133.17
4	B	2600	AGS	PB-O3B-PG	-3.36	120.88	133.17
4	D	4600	AGS	PB-O3B-PG	-3.23	121.35	133.17
4	C	3600	AGS	C4-C5-N7	-3.18	105.98	109.34
4	B	2600	AGS	C4-C5-N7	-3.11	106.05	109.34
4	E	5600	AGS	C4-C5-N7	-3.10	106.06	109.34
4	A	1600	AGS	PB-O3B-PG	-3.07	121.95	133.17
4	D	4600	AGS	C4-C5-N7	-3.05	106.11	109.34
4	F	6600	AGS	C4-C5-N7	-3.02	106.15	109.34
4	A	1600	AGS	C4-C5-N7	-3.01	106.15	109.34
4	C	3600	AGS	PB-O3B-PG	-2.96	122.32	133.17
4	F	6600	AGS	PB-O3B-PG	-2.89	122.58	133.17
5	E	5701	BCM	O2A-C2A-C1A	2.34	111.84	107.77
4	D	4600	AGS	C2'-C3'-C4'	2.10	106.68	102.61
4	B	2600	AGS	C4'-O4'-C1'	2.09	111.84	109.92
4	F	6600	AGS	C4'-O4'-C1'	2.06	111.81	109.92
4	C	3600	AGS	O3G-PG-O3B	2.05	111.47	104.64
5	D	4701	BCM	C2B-C2A-C3A	-2.04	106.56	109.93
4	A	1600	AGS	C4'-O4'-C1'	2.04	111.79	109.92
4	C	3600	AGS	C4'-O4'-C1'	2.04	111.79	109.92
4	E	5600	AGS	C4'-O4'-C1'	2.00	111.76	109.92

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3600	AGS	C5'-O5'-PA-O3A
4	D	4600	AGS	C5'-O5'-PA-O2A
4	E	5600	AGS	C5'-O5'-PA-O2A
4	E	5600	AGS	C5'-O5'-PA-O3A
4	F	6600	AGS	C5'-O5'-PA-O3A
5	B	2701	BCM	C1-C1A-C2A-O2A
5	B	2701	BCM	C1-C1A-C2A-C3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	2701	BCM	O1A-C1A-C2A-C2B
5	B	2701	BCM	O1A-C1A-C2A-O2A
5	C	3701	BCM	C1-C1A-C2A-C3A
5	C	3701	BCM	O1A-C1A-C2A-O2A
5	D	4701	BCM	N8-C1-C1A-O1A
5	D	4701	BCM	O2A-C2A-C3A-O3A
5	E	5701	BCM	N8-C1-C1A-O1A
5	E	5701	BCM	C1-C1A-C2A-C2B
5	E	5701	BCM	C1-C1A-C2A-O2A
5	E	5701	BCM	C1-C1A-C2A-C3A
5	E	5701	BCM	O1A-C1A-C2A-C2B
5	E	5701	BCM	O1A-C1A-C2A-O2A
5	E	5701	BCM	O1A-C1A-C2A-C3A
5	F	6701	BCM	C1-C1A-C2A-O2A
5	F	6701	BCM	C1-C1A-C2A-C3A
5	F	6701	BCM	O1A-C1A-C2A-C2B
5	F	6701	BCM	O1A-C1A-C2A-O2A
5	F	6701	BCM	O1A-C1A-C2A-C3A
4	C	3600	AGS	O4'-C4'-C5'-O5'
4	D	4600	AGS	O4'-C4'-C5'-O5'
4	E	5600	AGS	O4'-C4'-C5'-O5'
4	F	6600	AGS	O4'-C4'-C5'-O5'
4	D	4600	AGS	C3'-C4'-C5'-O5'
4	A	1600	AGS	O4'-C4'-C5'-O5'
4	B	2600	AGS	O4'-C4'-C5'-O5'
4	E	5600	AGS	C3'-C4'-C5'-O5'
4	C	3600	AGS	C3'-C4'-C5'-O5'
4	F	6600	AGS	C3'-C4'-C5'-O5'
4	A	1600	AGS	PA-O3A-PB-O1B
5	C	3701	BCM	O1A-C1A-C2A-C2B
4	B	2600	AGS	C3'-C4'-C5'-O5'
5	B	2701	BCM	C1-C1A-C2A-C2B
5	F	6701	BCM	C1-C1A-C2A-C2B
5	D	4701	BCM	C1A-C2A-C3A-O3A
5	D	4701	BCM	C2B-C2A-C3A-O3A
4	C	3600	AGS	C5'-O5'-PA-O2A
4	D	4600	AGS	C5'-O5'-PA-O1A
4	D	4600	AGS	C5'-O5'-PA-O3A
4	F	6600	AGS	C5'-O5'-PA-O2A
5	C	3701	BCM	C1-C1A-C2A-O2A
4	D	4600	AGS	PB-O3B-PG-O2G
5	B	2701	BCM	O1A-C1A-C2A-C3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	4600	AGS	PB-O3A-PA-O2A
4	E	5600	AGS	PB-O3A-PA-O2A
4	A	1600	AGS	C3'-C4'-C5'-O5'
4	F	6600	AGS	PB-O3A-PA-O2A

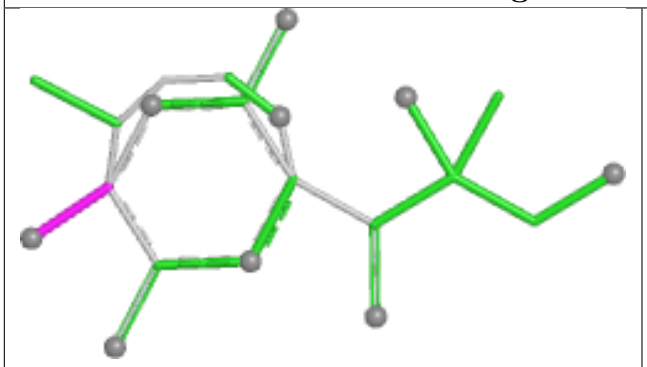
There are no ring outliers.

11 monomers are involved in 45 short contacts:

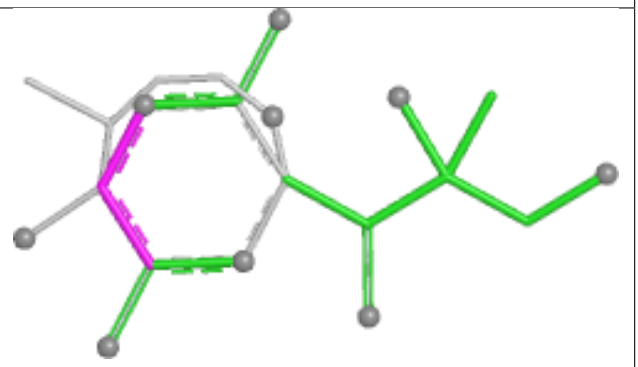
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2701	BCM	4	0
5	D	4701	BCM	5	0
4	C	3600	AGS	1	0
4	B	2600	AGS	2	0
4	F	6600	AGS	3	0
4	A	1600	AGS	1	0
5	C	3701	BCM	4	0
5	F	6701	BCM	7	0
4	E	5600	AGS	12	0
5	E	5701	BCM	2	0
4	D	4600	AGS	4	0

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.

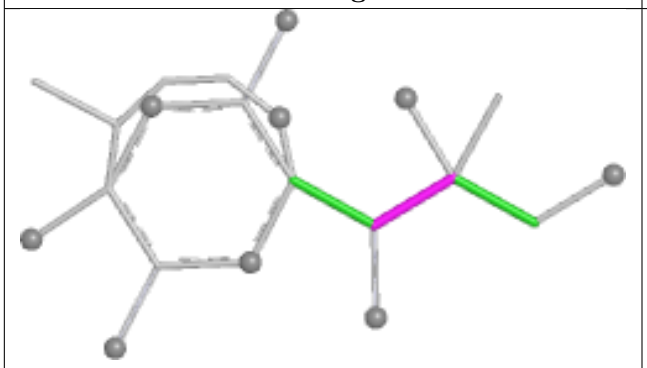
Ligand BCM B 2701



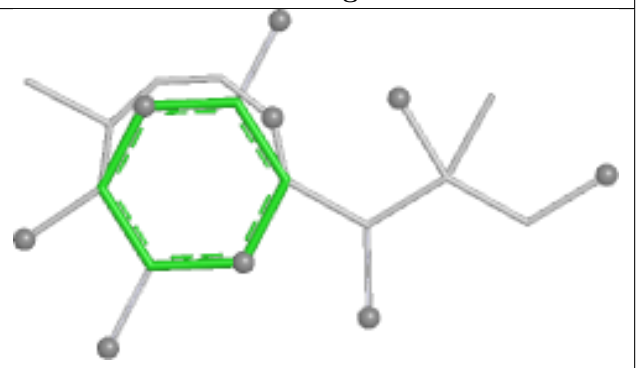
Bond lengths



Bond angles

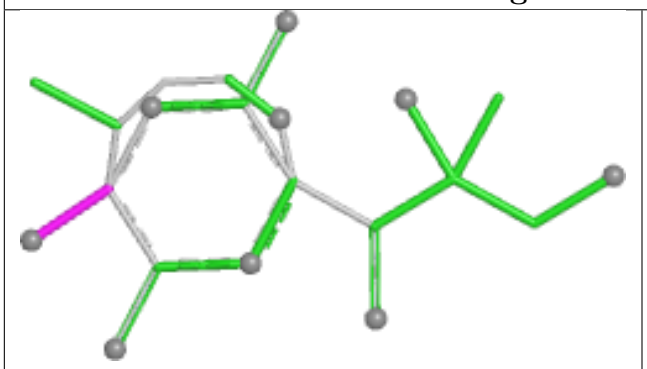


Torsions

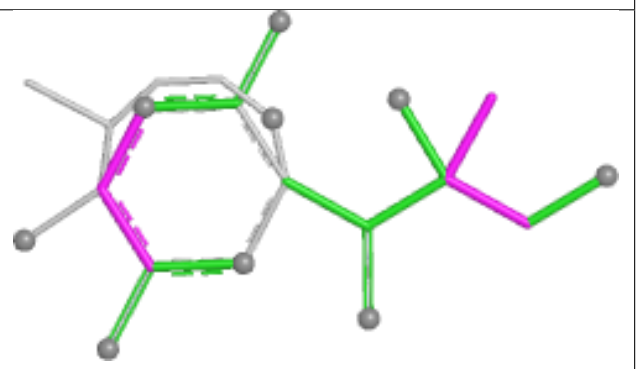


Rings

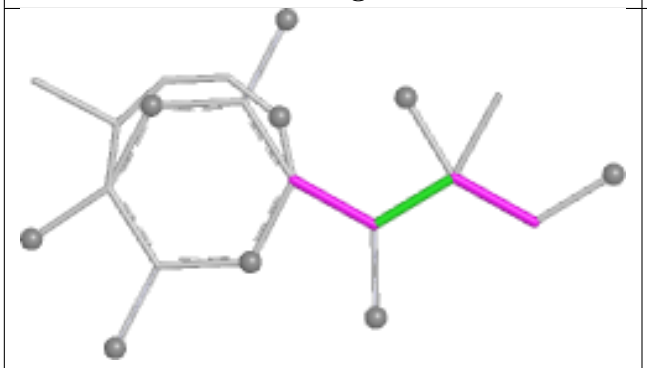
Ligand BCM D 4701



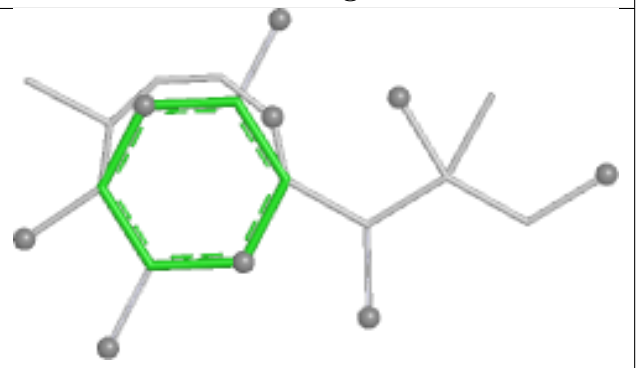
Bond lengths



Bond angles

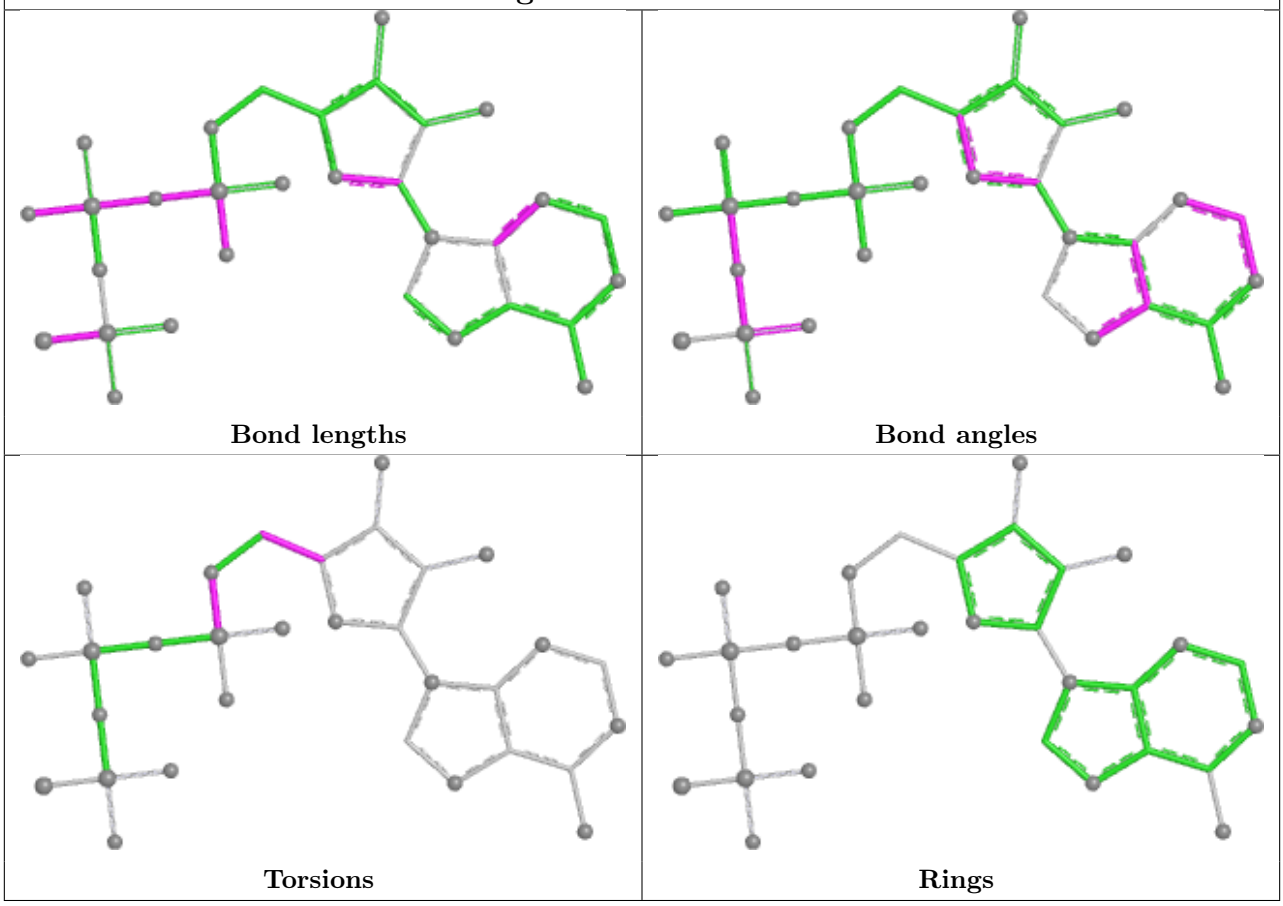


Torsions

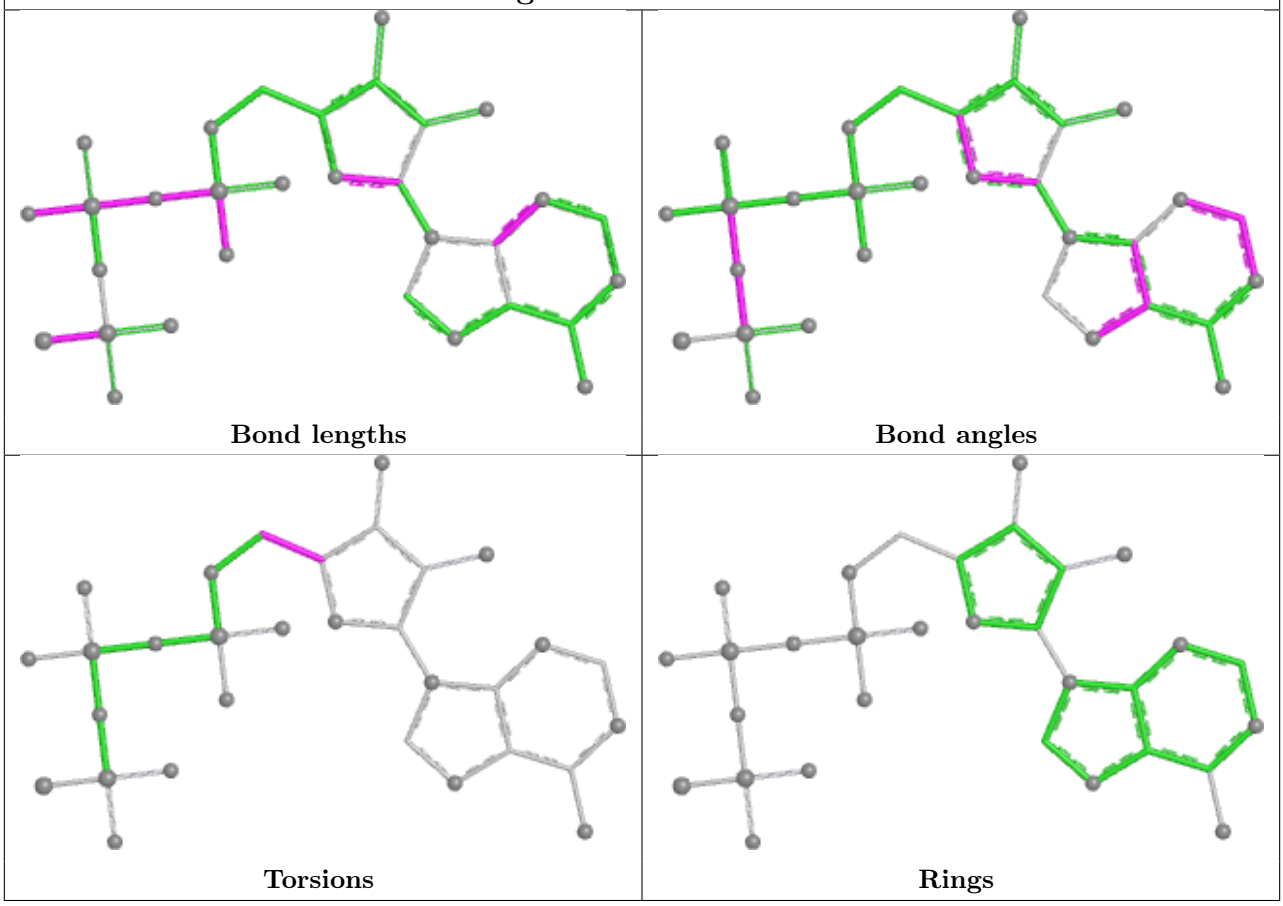


Rings

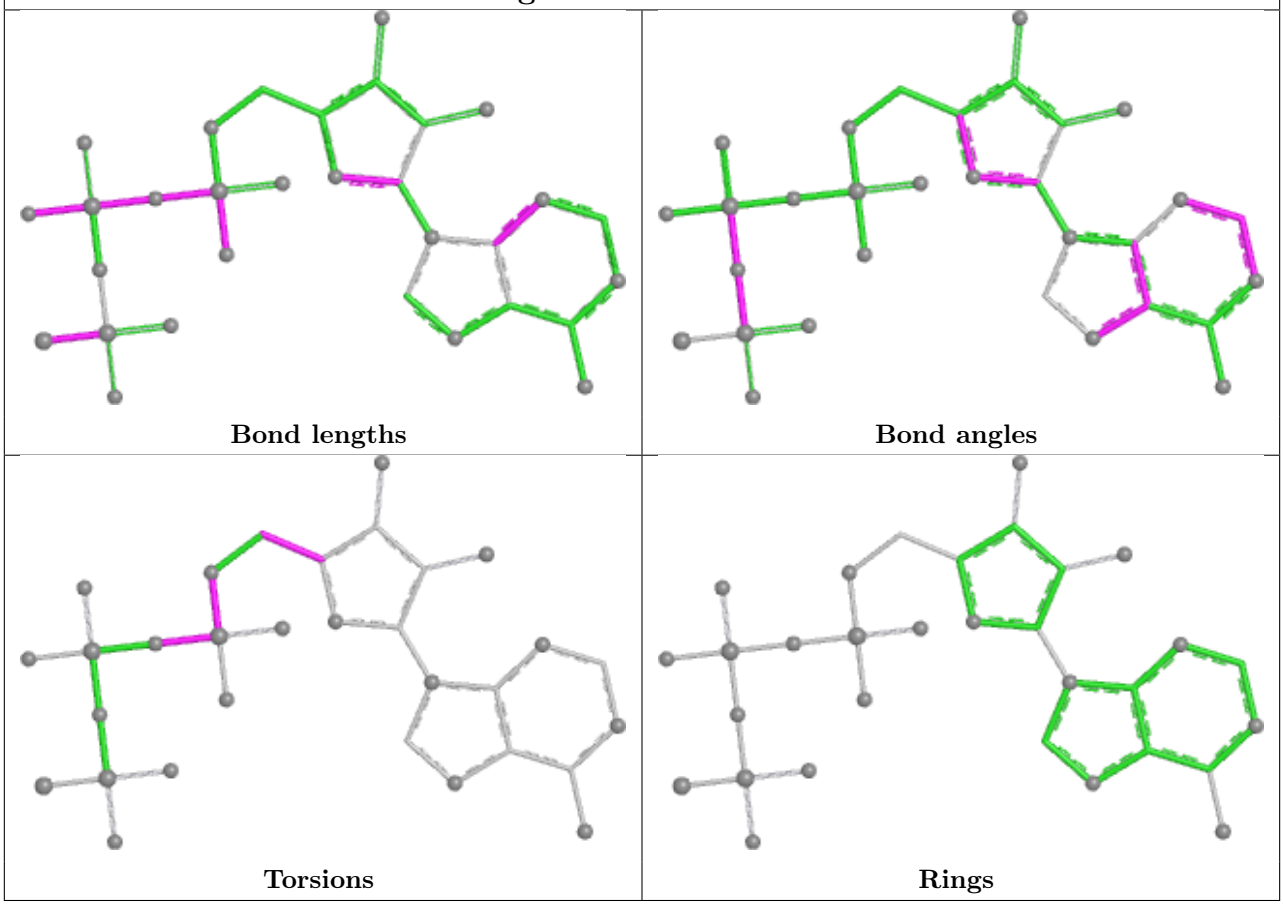
Ligand AGS C 3600



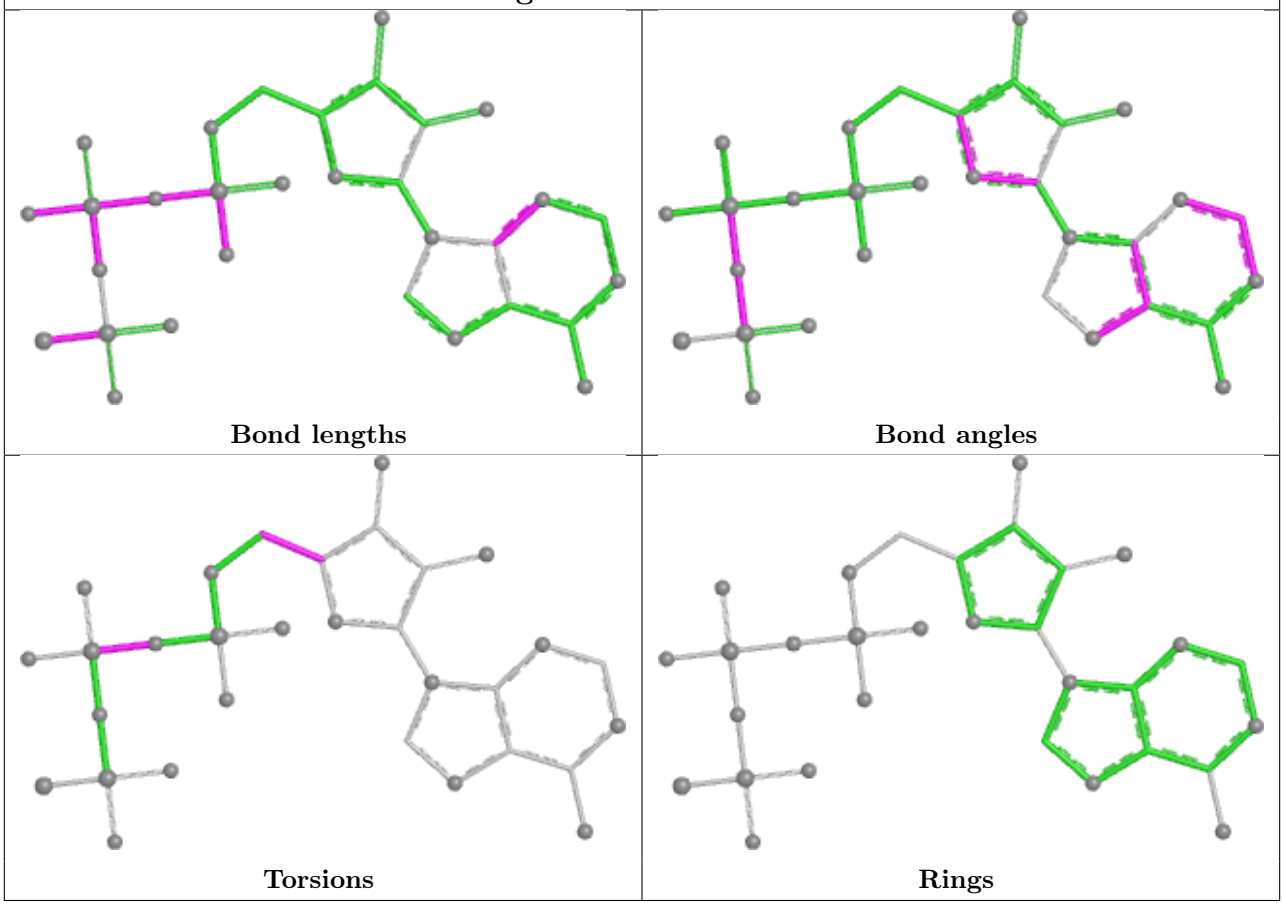
Ligand AGS B 2600



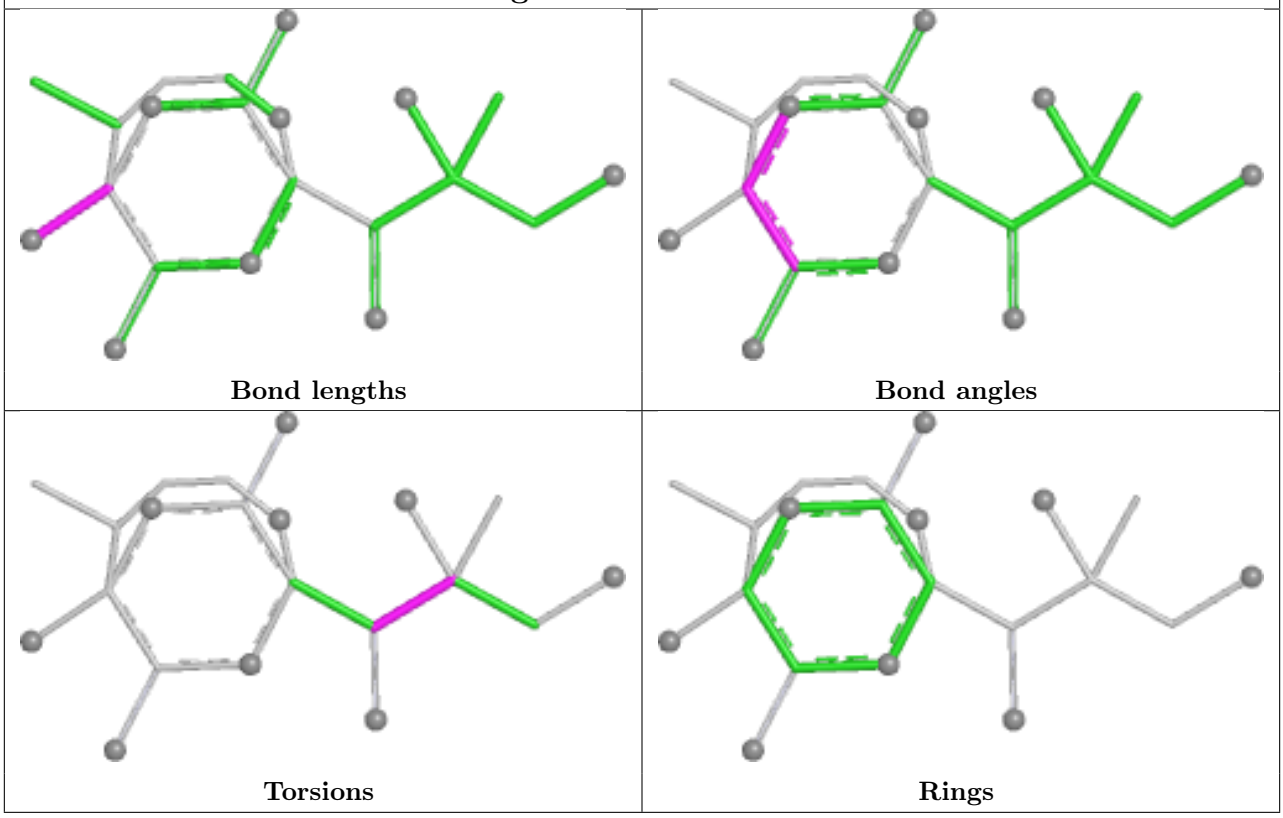
Ligand AGS F 6600



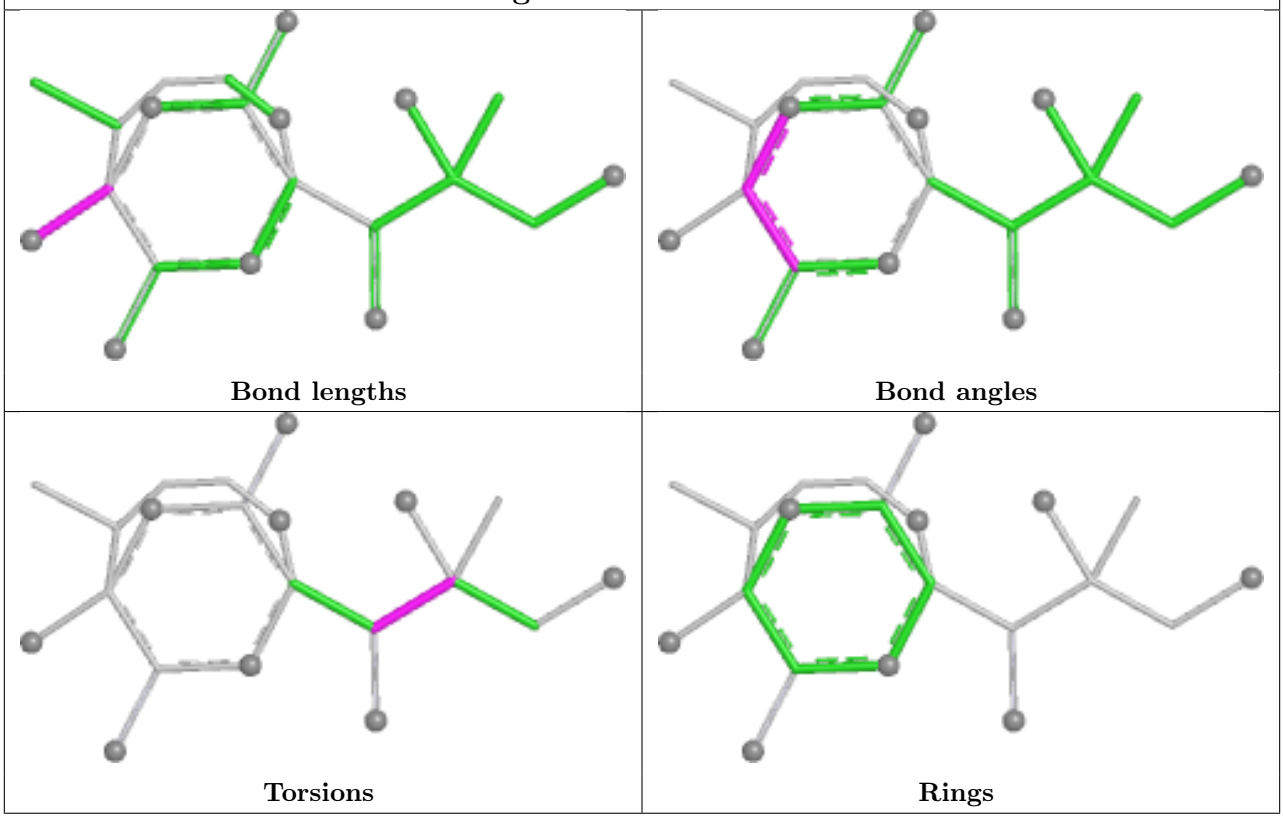
Ligand AGS A 1600



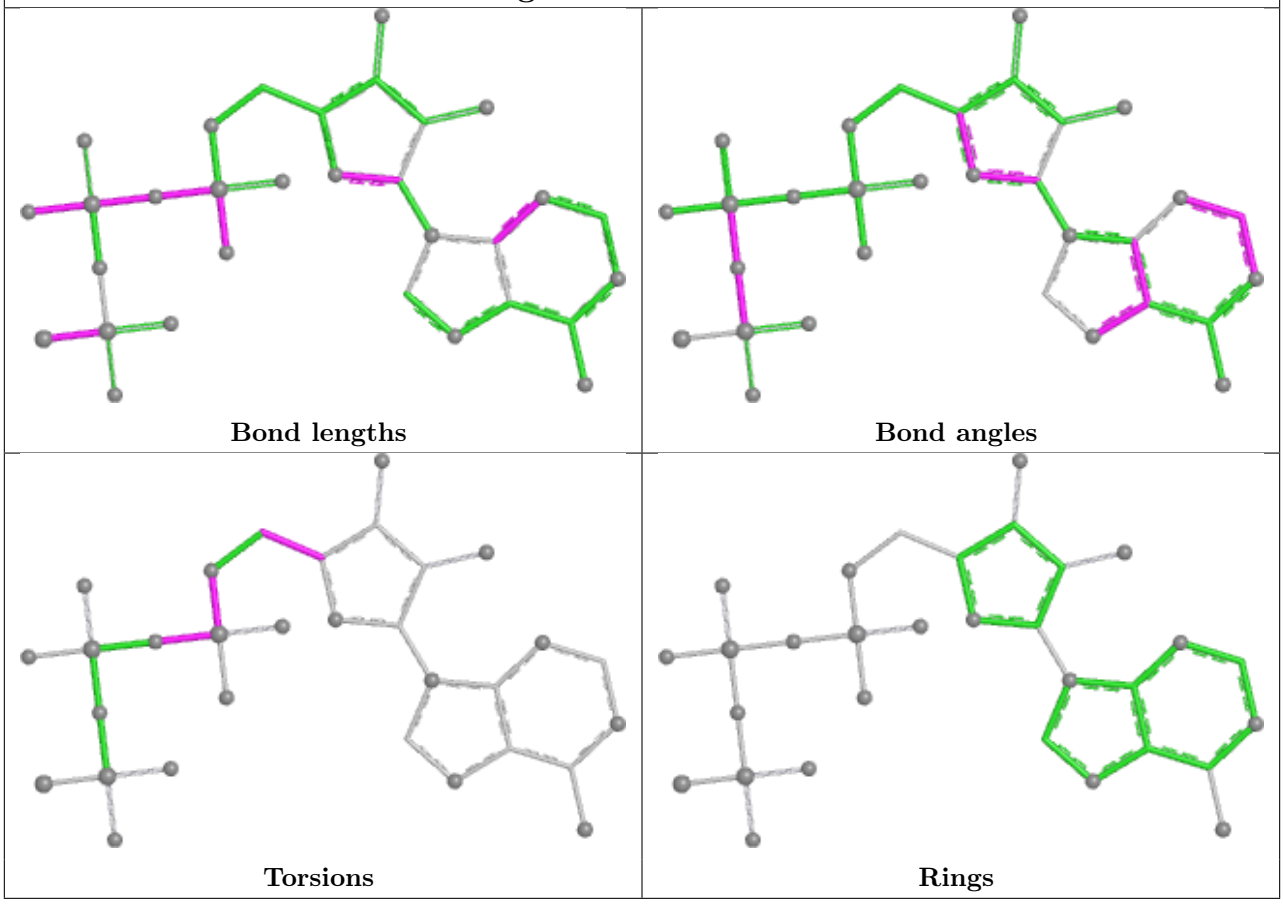
Ligand BCM C 3701



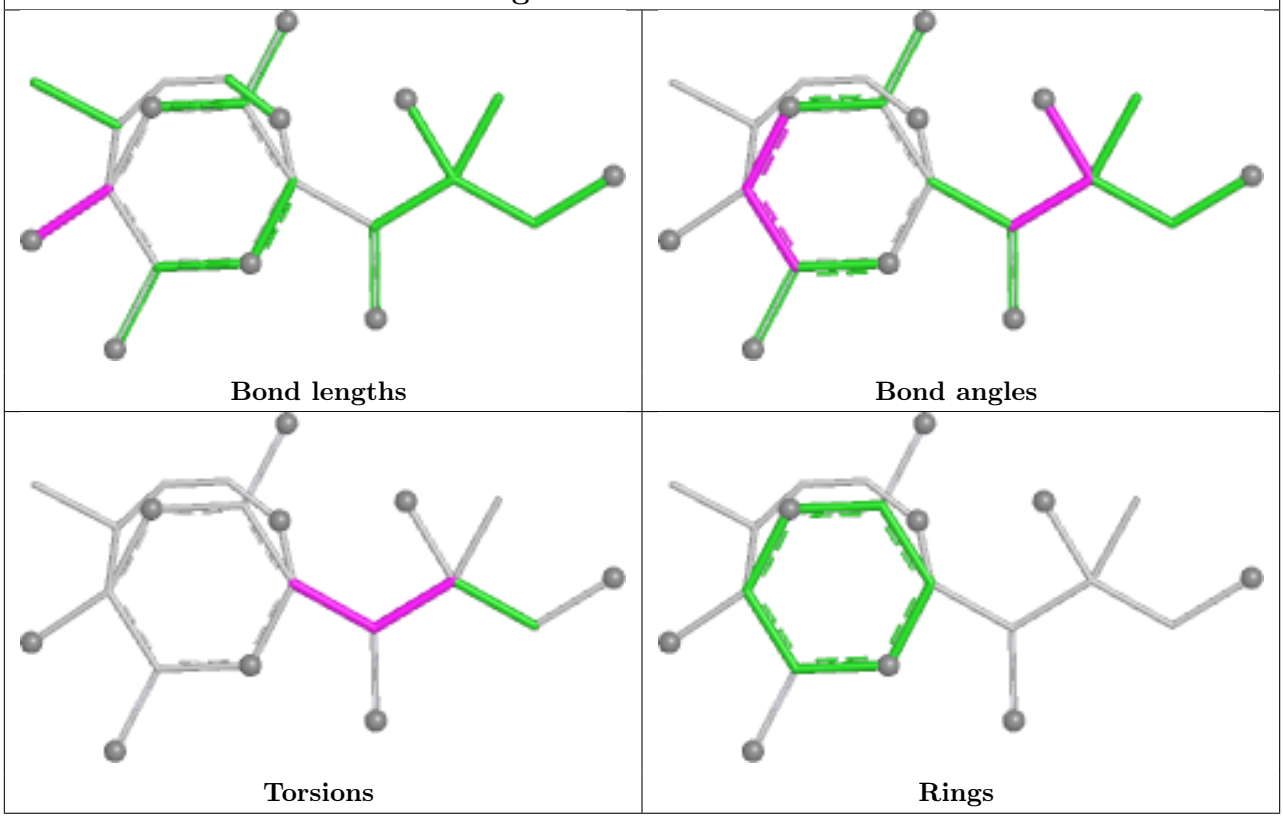
Ligand BCM F 6701



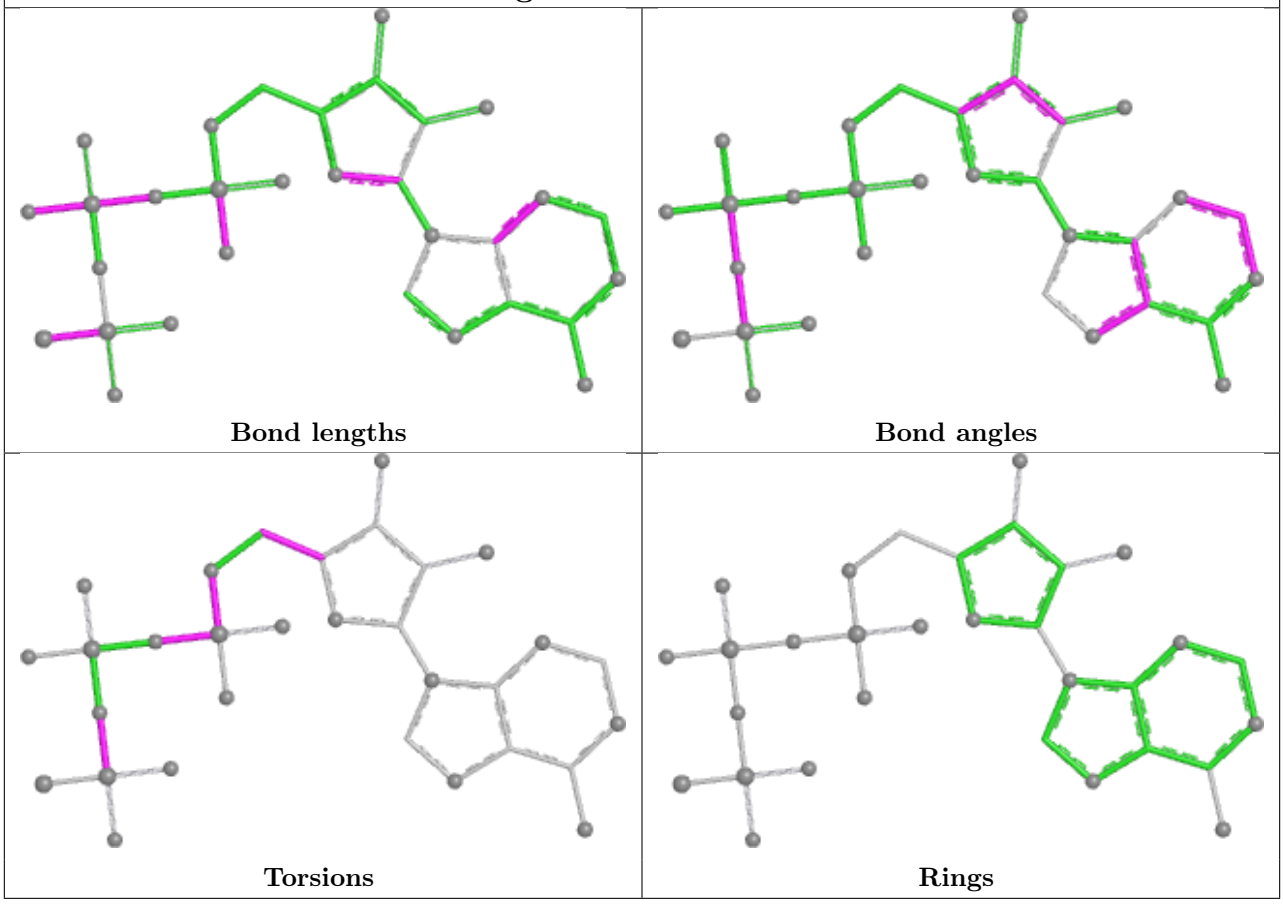
Ligand AGS E 5600



Ligand BCM E 5701



Ligand AGS D 4600



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	G	2/8 (25%)	7.68	2 (100%)	0	0	143, 143, 143, 143	0
1	H	2/8 (25%)	2.88	1 (50%)	0	0	143, 143, 143, 143	0
1	J	2/8 (25%)	2.03	1 (50%)	0	0	143, 143, 143, 143	0
1	K	2/8 (25%)	2.84	2 (100%)	0	0	143, 143, 143, 143	0
1	L	2/8 (25%)	2.84	1 (50%)	0	0	143, 143, 143, 143	0
1	M	2/8 (25%)	5.39	2 (100%)	0	0	143, 143, 143, 143	0
2	A	408/419 (97%)	0.25	18 (4%)	34	20	64, 96, 139, 140	0
2	B	408/419 (97%)	0.21	23 (5%)	24	12	56, 92, 125, 139	0
2	C	408/419 (97%)	0.07	12 (2%)	51	35	46, 68, 120, 124	0
2	D	408/419 (97%)	0.10	5 (1%)	79	68	52, 79, 114, 138	0
2	E	407/419 (97%)	0.10	11 (2%)	54	38	53, 80, 122, 139	0
2	F	408/419 (97%)	0.13	9 (2%)	62	47	60, 88, 128, 138	0
All	All	2459/2562 (95%)	0.16	87 (3%)	44	27	46, 85, 137, 143	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	C	7.8
1	G	1	U	7.6
1	M	2	C	6.7
2	C	138	PRO	6.5
2	B	415	MET	5.3
2	F	284	VAL	5.2
2	C	1	MET	4.8
2	B	414	GLU	4.6
2	A	412	PHE	4.4
2	E	47	GLU	4.4
2	B	413	PHE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	1	U	4.1
2	B	8	ASN	4.0
2	E	410	ASP	4.0
2	B	417	LYS	4.0
1	H	2	C	3.9
2	A	415	MET	3.9
2	C	406	THR	3.8
1	L	1	U	3.7
2	A	50	PHE	3.6
2	F	45	SER	3.6
2	D	413	PHE	3.6
2	B	407	LYS	3.5
2	B	46	GLY	3.5
2	E	152	GLY	3.4
1	K	1	U	3.4
2	B	62	PHE	3.2
2	B	400	ILE	3.2
2	F	48	ASP	3.1
2	D	23	LEU	3.0
2	B	61	GLY	3.0
2	A	202	CYS	3.0
2	A	155	GLU	2.9
2	A	138	PRO	2.8
2	B	352	LYS	2.8
2	C	15	ILE	2.8
2	E	84	SER	2.8
2	B	60	ASP	2.8
2	F	21	MET	2.8
2	B	140	HIS	2.8
2	A	417	LYS	2.8
2	A	48	ASP	2.7
2	A	140	HIS	2.7
2	C	21	MET	2.6
2	D	99	GLY	2.6
2	A	346	SER	2.6
2	D	84	SER	2.6
2	C	46	GLY	2.5
2	A	414	GLU	2.5
2	C	324	GLY	2.5
2	F	140	HIS	2.4
2	E	412	PHE	2.4
2	A	125	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	154	THR	2.4
2	C	60	ASP	2.4
2	E	48	ASP	2.4
2	F	129	ASN	2.3
2	F	355	PHE	2.3
2	B	23	LEU	2.3
1	K	2	C	2.3
2	E	60	ASP	2.3
2	E	44	LYS	2.3
2	E	140	HIS	2.2
2	A	16	THR	2.2
2	B	21	MET	2.2
2	D	62	PHE	2.2
2	C	19	GLU	2.2
2	B	416	MET	2.2
2	A	317	ALA	2.1
2	F	52	ASP	2.1
1	J	2	C	2.1
2	B	152	GLY	2.1
2	A	12	SER	2.1
2	B	280	ALA	2.1
2	A	88	ARG	2.1
2	B	142	ASN	2.1
2	F	285	LEU	2.1
2	C	12	SER	2.1
2	B	64	PHE	2.1
2	B	378	GLN	2.0
2	B	365	THR	2.0
2	C	365	THR	2.0
2	E	406	THR	2.0
2	A	224	LYS	2.0
2	B	198	ASN	2.0
2	E	365	THR	2.0
2	C	59	GLN	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)

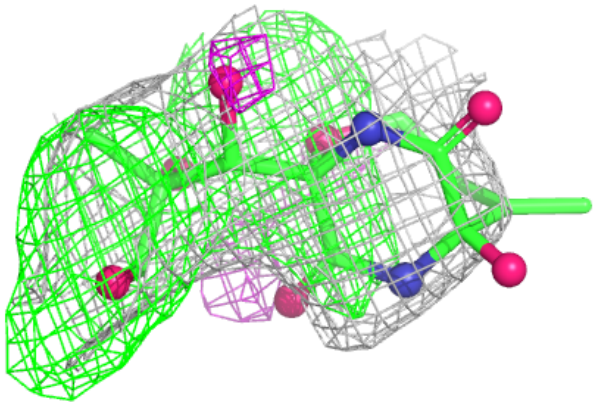
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

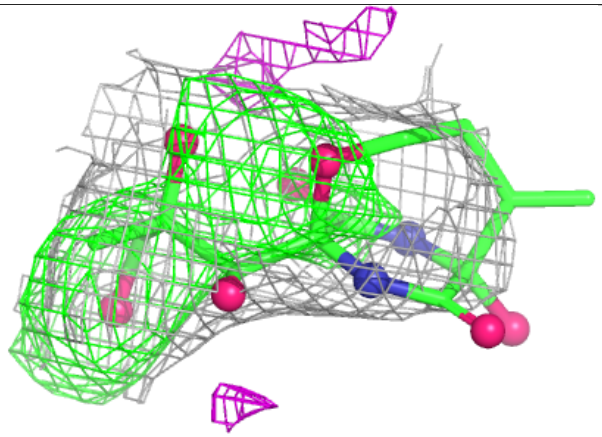
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	3601	1/1	0.46	0.37	89,89,89,89	0
5	BCM	F	6701	21/21	0.58	0.59	78,78,79,79	0
4	AGS	C	3600	31/31	0.69	0.41	93,95,104,104	0
3	MG	A	1601	1/1	0.72	0.20	89,89,89,89	0
3	MG	E	5601	1/1	0.72	0.32	82,82,82,82	0
5	BCM	D	4701	21/21	0.77	0.48	77,77,77,77	0
5	BCM	C	3701	21/21	0.77	0.40	77,77,77,77	0
4	AGS	B	2600	31/31	0.78	0.33	93,96,104,104	0
4	AGS	F	6600	31/31	0.79	0.42	92,95,104,104	0
5	BCM	E	5701	21/21	0.80	0.46	86,86,86,86	0
5	BCM	B	2701	21/21	0.81	0.26	76,76,76,76	0
4	AGS	A	1600	31/31	0.83	0.22	93,95,104,104	0
4	AGS	D	4600	31/31	0.84	0.30	93,95,103,104	0
4	AGS	E	5600	31/31	0.86	0.23	93,95,104,104	0
3	MG	F	6601	1/1	0.88	0.18	69,69,69,69	0
3	MG	B	2601	1/1	0.93	0.61	85,85,85,85	0
3	MG	D	4601	1/1	0.94	0.51	70,70,70,70	0

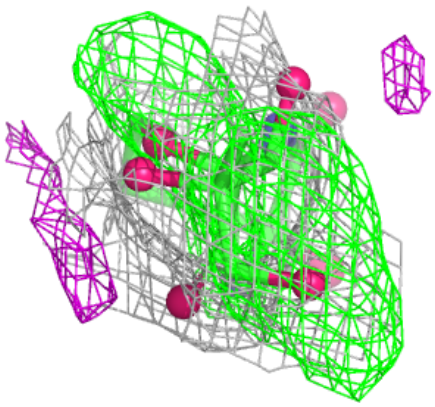
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BCM F 6701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

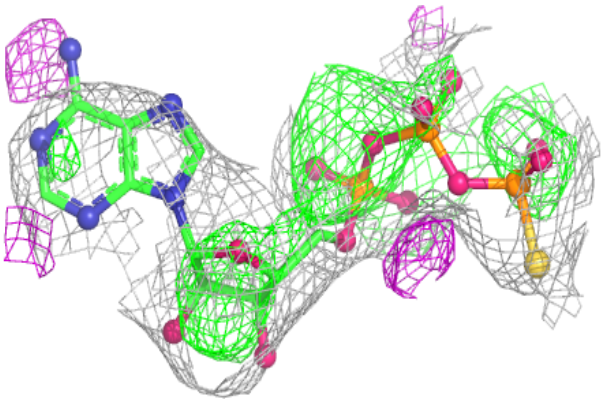


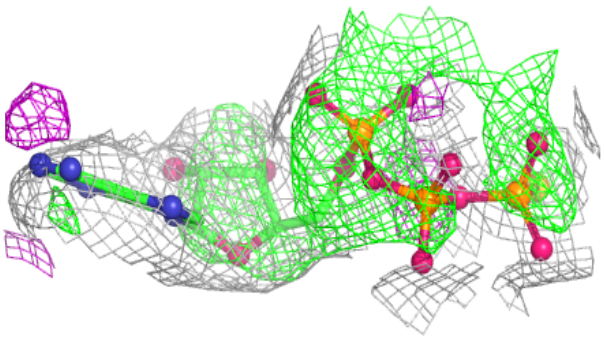


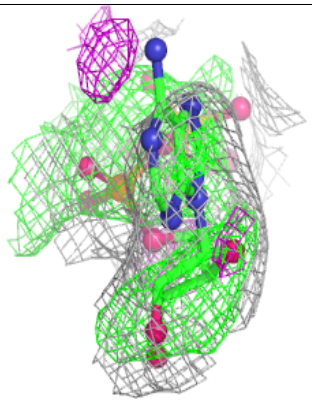


Electron density around AGS C 3600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

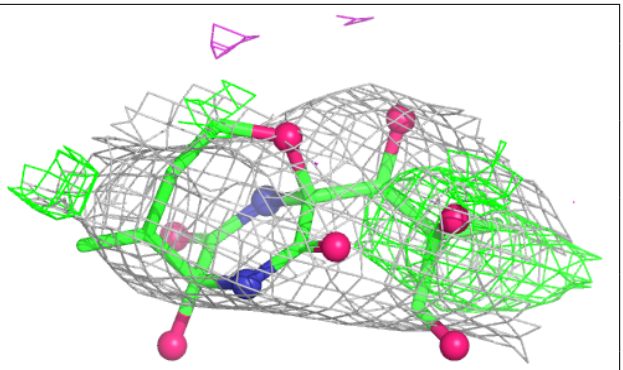


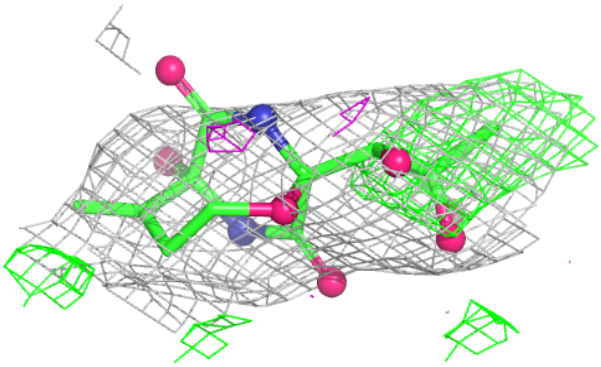


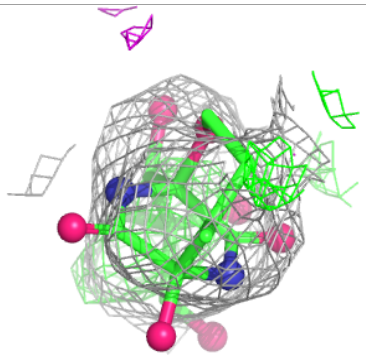


Electron density around BCM D 4701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

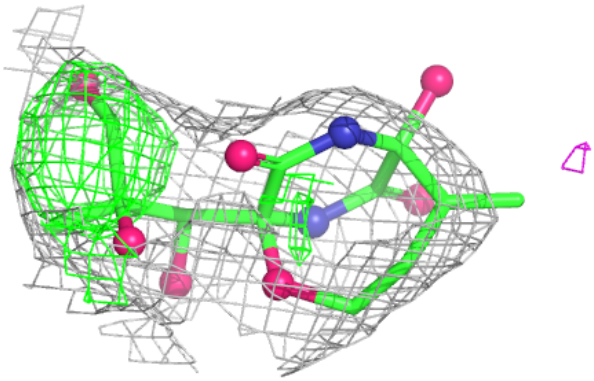


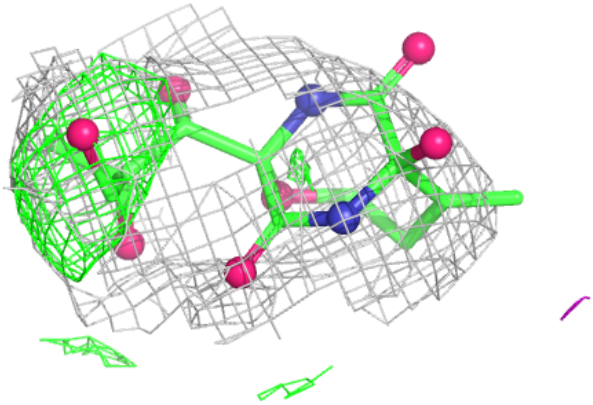


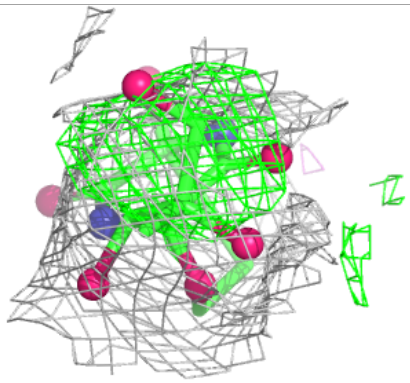


Electron density around BCM C 3701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

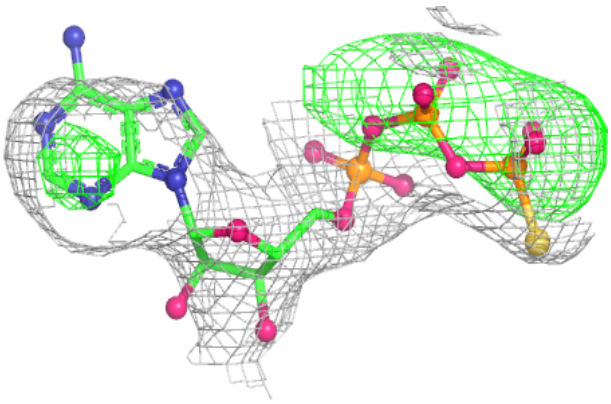


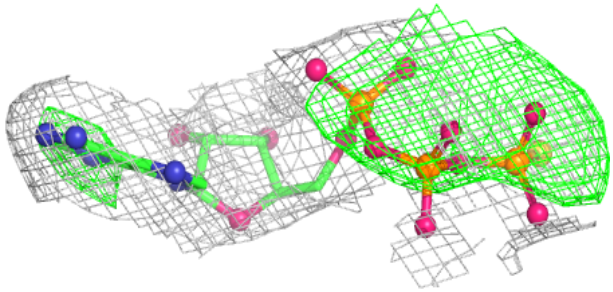


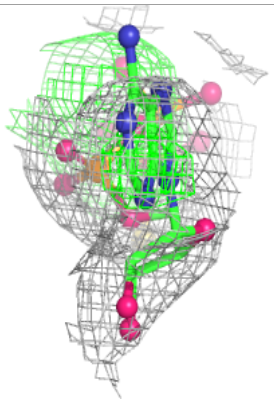


Electron density around AGS B 2600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

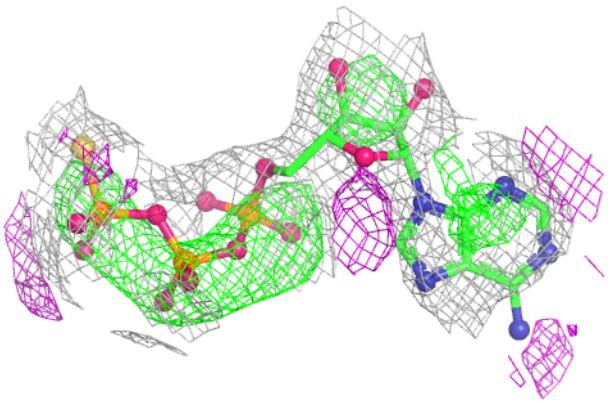


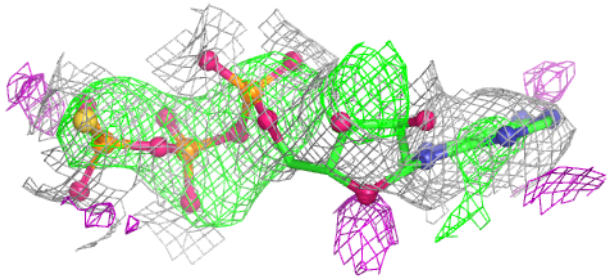


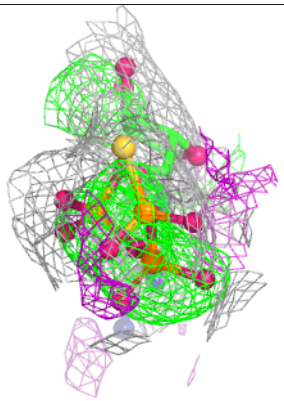


Electron density around AGS F 6600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

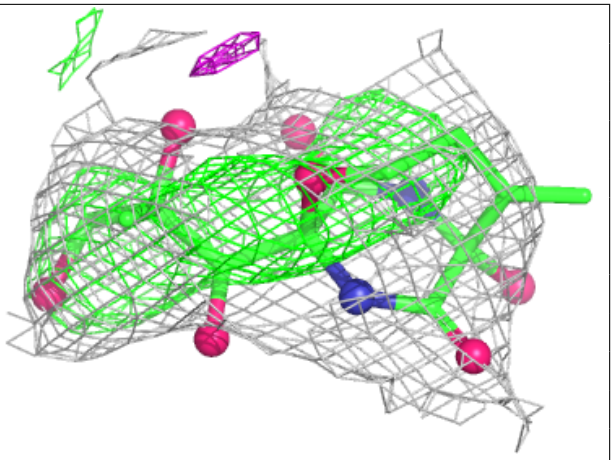


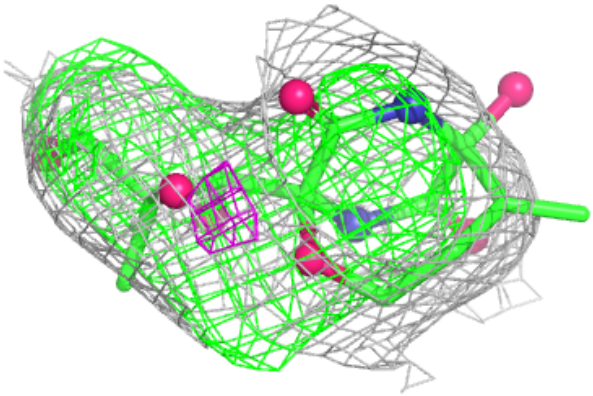


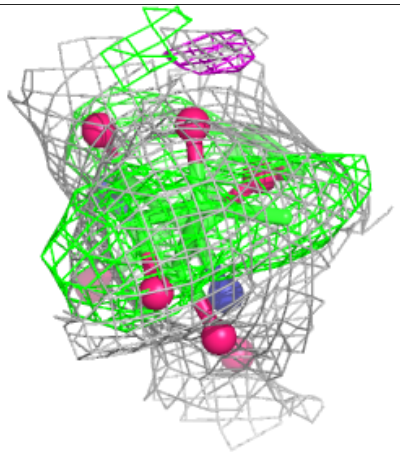


Electron density around BCM E 5701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

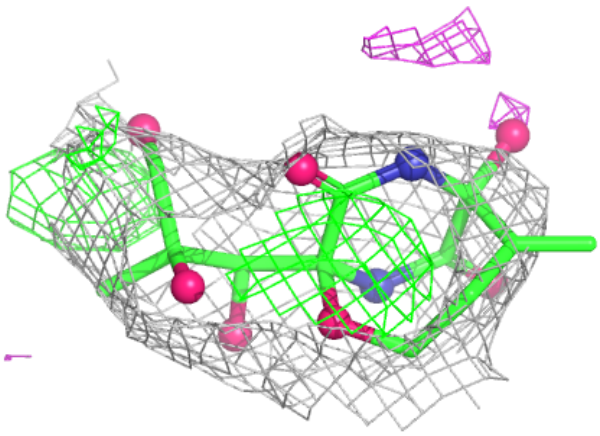


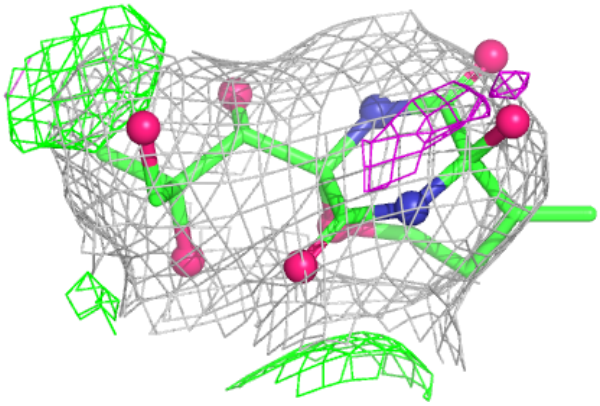


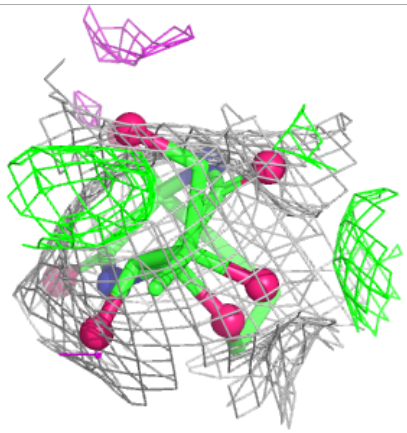


Electron density around BCM B 2701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

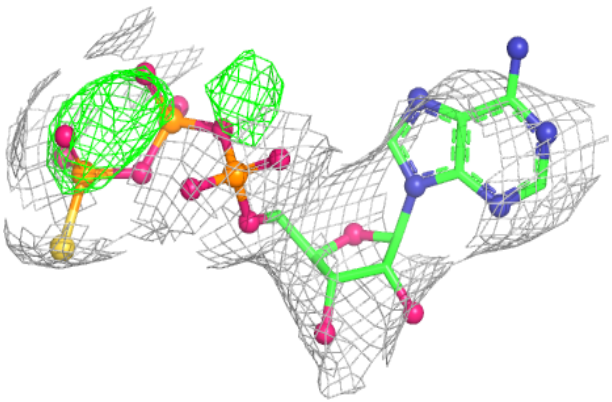


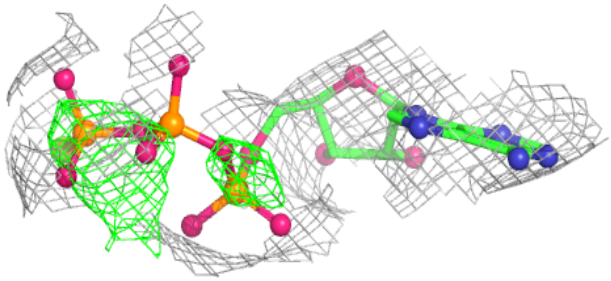


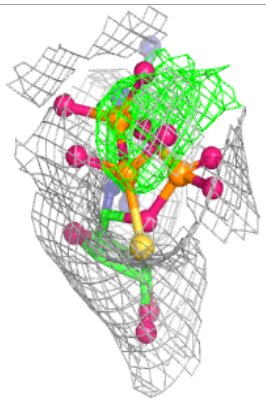


Electron density around AGS A 1600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

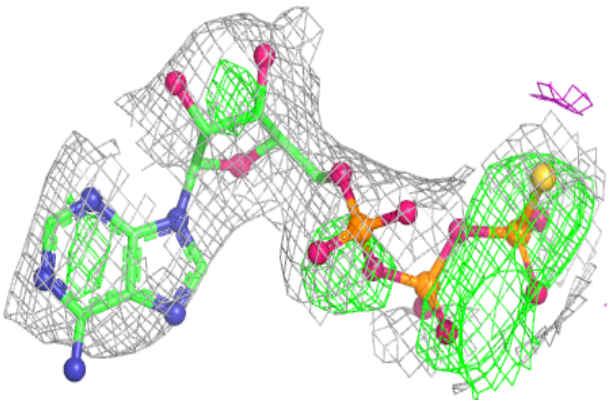


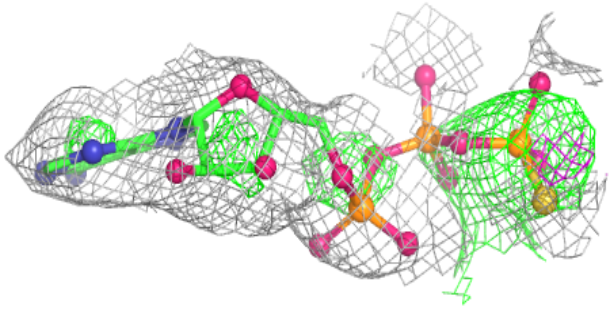


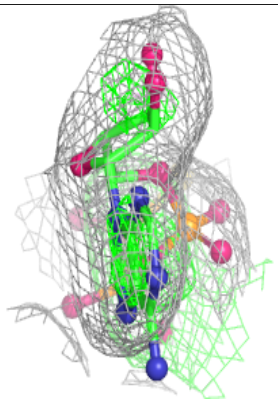


Electron density around AGS D 4600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

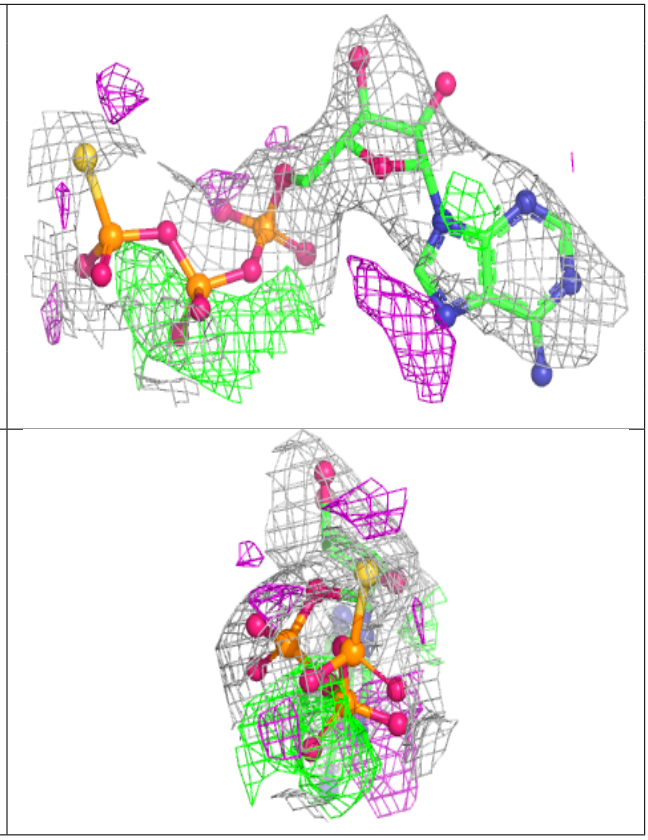






Electron density around AGS E 5600:

$2mF_o$-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.