Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 11:09 AM EST

PDB ID	:	1XPR
Title	:	Structural mechanism of inhibition of the Rho transcription termination factor by the antibiotic 5a-formylbicyclomycin (FB)
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:

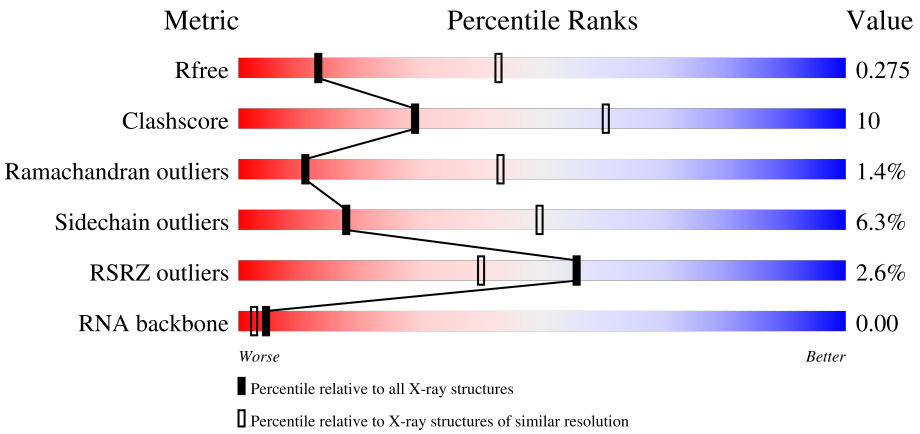
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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

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Mol	Chain	Length	Quality of chain
1	L	8	25% 75%
1	M	8	25% 12% 12% 75%
2	A	419	4% 69% 25%
2	B	419	2% 69% 25%
2	C	419	75% 21%
2	D	419	2% 74% 21%
2	E	419	% 68% 26%
2	F	419	3% 74% 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	B	2600	-	-	X	-
4	AGS	C	3600	-	-	-	X
4	AGS	D	4600	-	-	X	X
4	AGS	E	5600	-	-	-	X
4	AGS	F	6600	-	-	-	X
5	FB	B	2701	-	-	-	X
5	FB	D	4701	-	-	-	X
5	FB	E	5701	-	-	-	X
5	FB	F	6701	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19814 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	39	17	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	40	18	5	15	2	0	0	0

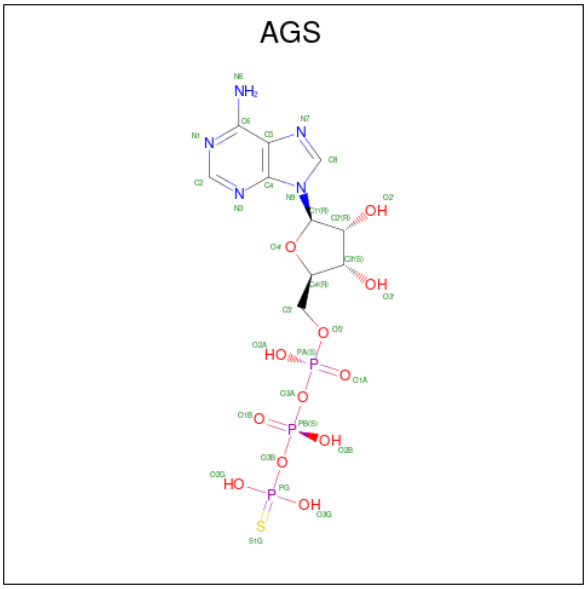
- Molecule 2 is a protein called Rho transcription termination factor.

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

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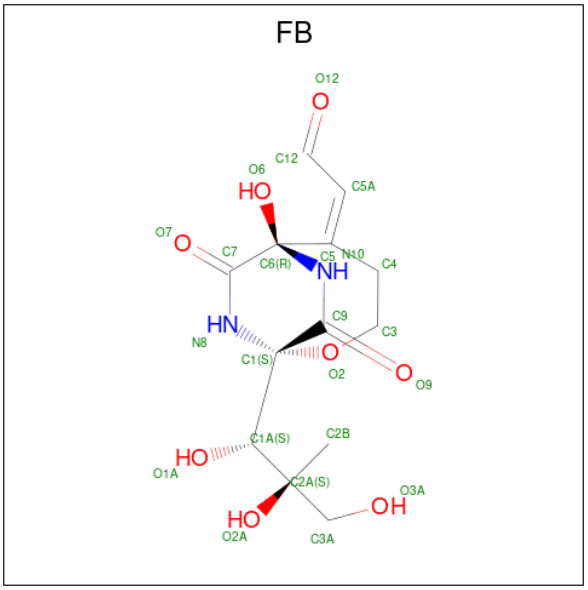
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	F	1	31	10	5	12	3	1	0	0

- Molecule 5 is 5A-FORMYLBICYCLOMYCIN (three-letter code: FB) (formula: $C_{13}H_{18}N_2O_8$).



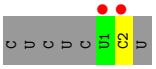
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	23	13	2	8	0	0
5	C	1	23	13	2	8	0	0
5	D	1	23	13	2	8	0	0
5	E	1	23	13	2	8	0	0
5	F	1	23	13	2	8	0	0

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.

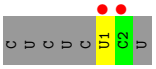
• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain G:



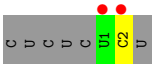
• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain M:



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

Chain H:

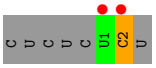


• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain J:

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

Chain K:

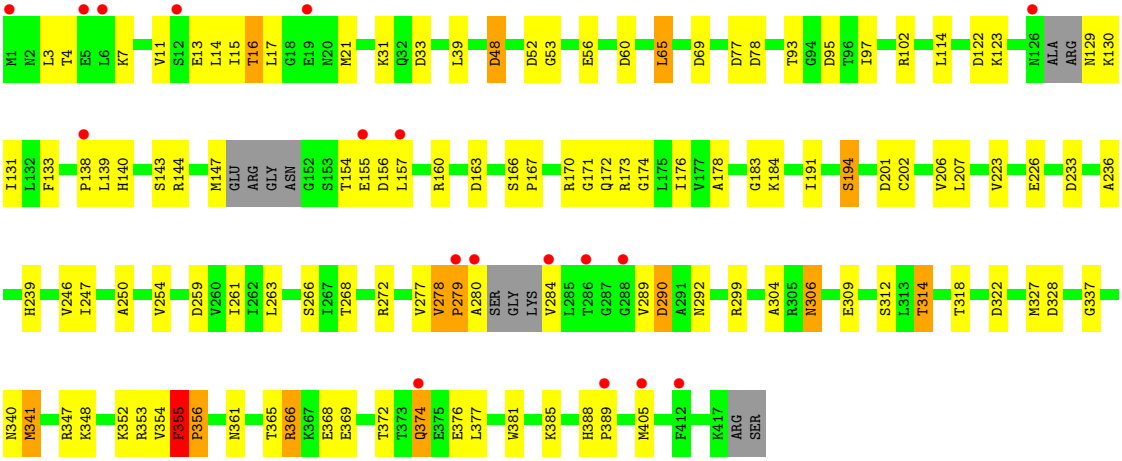


• Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain L:

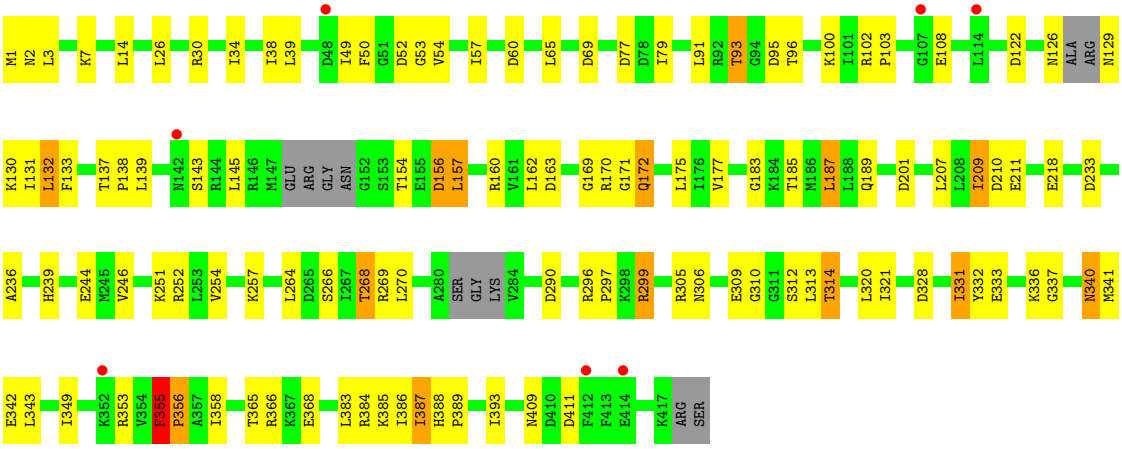
• Molecule 2: Rho transcription termination factor

Chain A:



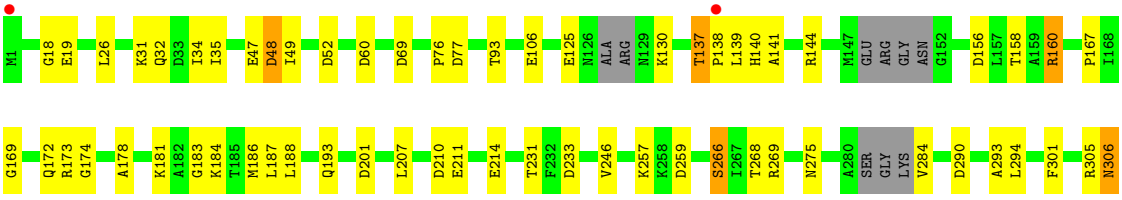
• Molecule 2: Rho transcription termination factor

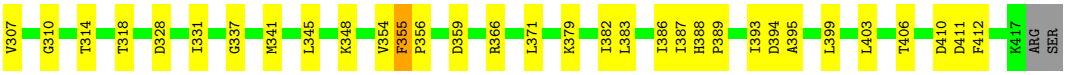
Chain B:



• Molecule 2: Rho transcription termination factor

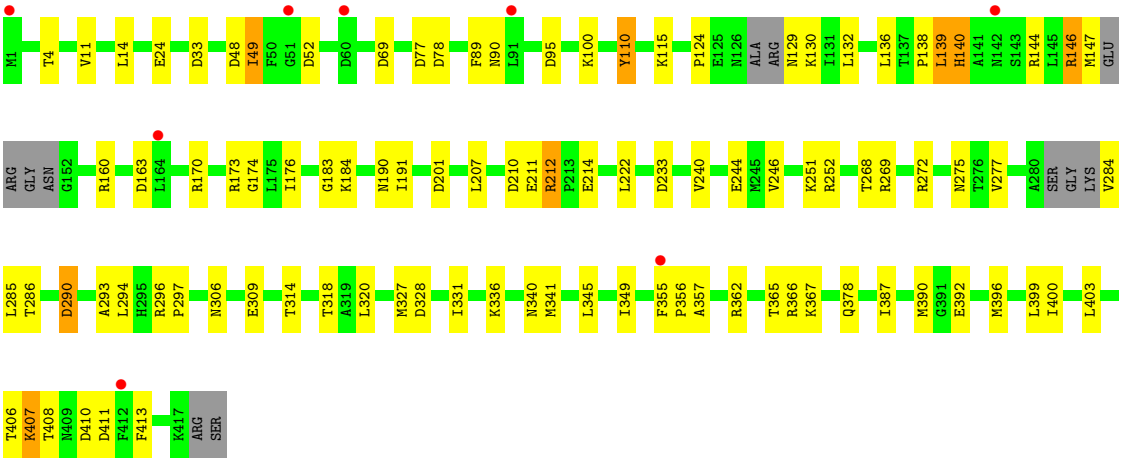
Chain C:





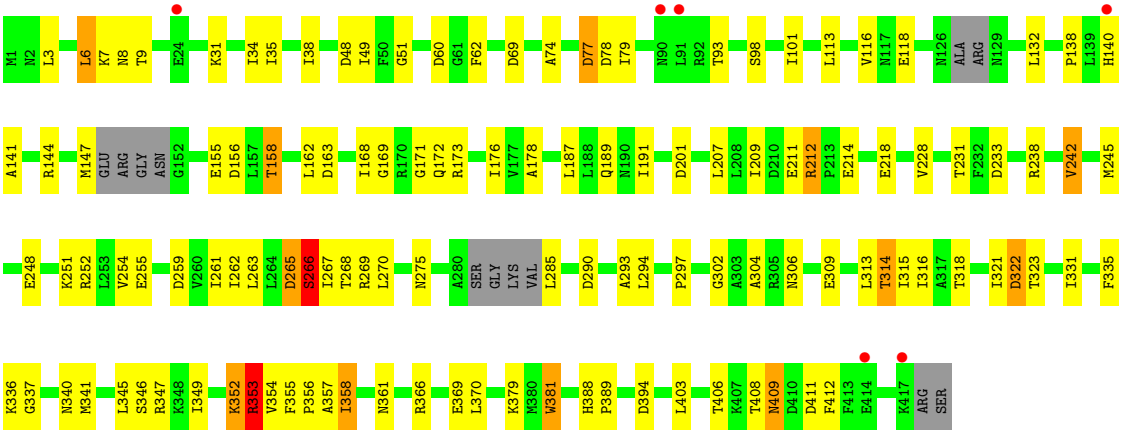
• Molecule 2: Rho transcription termination factor

Chain D:



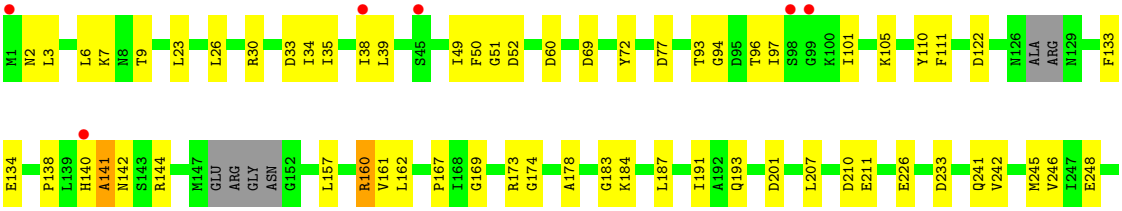
• Molecule 2: Rho transcription termination factor

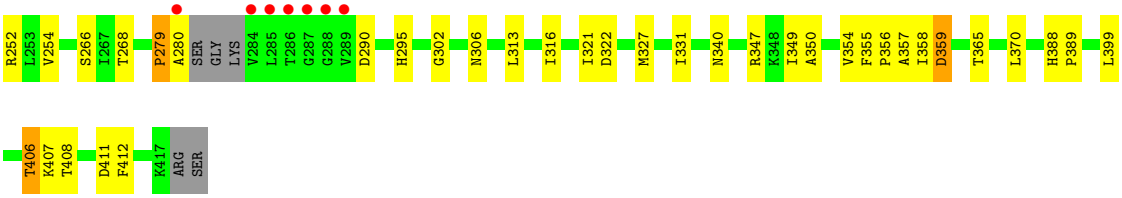
Chain E:



• Molecule 2: Rho transcription termination factor

Chain F:




R252
L253
V254
S266
I267
T268
P279
A280
SER
GLY
LYS
V284
L285
T286
G287
G288
V289
D290
H295
G302
N306
L313
I316
I321
D322
M327
I331
N340
R347
K348
I349
A350
V354
F355
P356
A357
I358
D359
T365
L370
H388
P389
L399
T406
K407
T408
D411
F412
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	210.53Å 109.68Å 160.05Å 90.00° 108.16° 90.00°	Depositor
Resolution (Å)	20.00 – 3.15 39.26 – 3.10	Depositor EDS
% Data completeness (in resolution range)	86.5 (20.00-3.15) 85.8 (39.26-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.274 , 0.296 0.269 , 0.275	Depositor DCC
R_{free} test set	2754 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	100.9	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 66.6	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	0.91	EDS
Total number of atoms	19814	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, FB, AGS

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	0.73	0/43	1.04	0/64
1	H	0.79	0/43	1.15	0/64
1	J	0.70	0/43	1.02	0/64
1	K	0.72	0/43	0.94	0/64
1	L	0.79	0/43	1.52	0/64
1	M	0.75	0/41	1.12	0/60
2	A	0.31	0/3256	0.65	14/4383 (0.3%)
2	B	0.31	0/3259	0.65	10/4387 (0.2%)
2	C	0.30	0/3259	0.63	12/4387 (0.3%)
2	D	0.30	0/3259	0.64	14/4387 (0.3%)
2	E	0.30	0/3252	0.63	11/4377 (0.3%)
2	F	0.30	0/3259	0.64	10/4387 (0.2%)
All	All	0.31	0/19800	0.65	71/26688 (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	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	60	ASP	CB-CG-OD2	6.32	123.98	118.30
2	D	77	ASP	CB-CG-OD2	6.20	123.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	77	ASP	CB-CG-OD2	5.99	123.69	118.30
2	B	77	ASP	CB-CG-OD2	5.97	123.67	118.30
2	E	163	ASP	CB-CG-OD2	5.91	123.62	118.30
2	A	48	ASP	CB-CG-OD2	5.89	123.60	118.30
2	E	233	ASP	CB-CG-OD2	5.88	123.59	118.30
2	C	52	ASP	CB-CG-OD2	5.84	123.56	118.30
2	A	322	ASP	CB-CG-OD2	5.84	123.55	118.30
2	D	210	ASP	CB-CG-OD2	5.82	123.54	118.30
2	D	410	ASP	CB-CG-OD2	5.79	123.51	118.30
2	F	33	ASP	CB-CG-OD2	5.77	123.49	118.30
2	E	48	ASP	CB-CG-OD2	5.75	123.47	118.30
2	B	233	ASP	CB-CG-OD2	5.74	123.46	118.30
2	E	78	ASP	CB-CG-OD2	5.74	123.46	118.30
2	A	33	ASP	CB-CG-OD2	5.72	123.45	118.30
2	A	77	ASP	CB-CG-OD2	5.71	123.44	118.30
2	F	233	ASP	CB-CG-OD2	5.71	123.44	118.30
2	E	156	ASP	CB-CG-OD2	5.69	123.42	118.30
2	A	78	ASP	CB-CG-OD2	5.67	123.40	118.30
2	E	77	ASP	CB-CG-OD2	5.66	123.39	118.30
2	F	52	ASP	CB-CG-OD2	5.63	123.36	118.30
2	A	60	ASP	CB-CG-OD2	5.56	123.30	118.30
2	F	69	ASP	CB-CG-OD2	5.51	123.26	118.30
2	F	77	ASP	CB-CG-OD2	5.50	123.25	118.30
2	C	69	ASP	CB-CG-OD2	5.42	123.18	118.30
2	E	69	ASP	CB-CG-OD2	5.36	123.12	118.30
2	A	69	ASP	CB-CG-OD2	5.31	123.08	118.30
2	E	265	ASP	CB-CG-OD2	5.31	123.08	118.30
2	D	95	ASP	CB-CG-OD2	5.26	123.03	118.30
2	A	233	ASP	CB-CG-OD2	5.26	123.03	118.30
2	B	95	ASP	CB-CG-OD2	5.25	123.03	118.30
2	C	210	ASP	CB-CG-OD2	5.23	123.01	118.30
2	D	78	ASP	CB-CG-OD2	5.19	122.97	118.30
2	D	48	ASP	CB-CG-OD2	5.18	122.96	118.30
2	A	290	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	210	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	69	ASP	CB-CG-OD2	5.17	122.95	118.30
2	C	60	ASP	CB-CG-OD2	5.16	122.94	118.30
2	A	163	ASP	CB-CG-OD2	5.16	122.94	118.30
2	C	328	ASP	CB-CG-OD2	5.14	122.92	118.30
2	C	201	ASP	CB-CG-OD2	5.12	122.91	118.30
2	A	201	ASP	CB-CG-OD2	5.11	122.90	118.30
2	A	95	ASP	CB-CG-OD2	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	201	ASP	CB-CG-OD2	5.11	122.90	118.30
2	A	328	ASP	CB-CG-OD2	5.10	122.89	118.30
2	D	290	ASP	CB-CG-OD2	5.09	122.89	118.30
2	D	163	ASP	CB-CG-OD2	5.09	122.88	118.30
2	D	33	ASP	CB-CG-OD2	5.09	122.88	118.30
2	B	163	ASP	CB-CG-OD2	5.08	122.87	118.30
2	E	394	ASP	CB-CG-OD2	5.08	122.87	118.30
2	F	201	ASP	CB-CG-OD2	5.08	122.87	118.30
2	F	210	ASP	CB-CG-OD2	5.07	122.87	118.30
2	C	259	ASP	CB-CG-OD2	5.06	122.86	118.30
2	B	328	ASP	CB-CG-OD2	5.06	122.85	118.30
2	C	359	ASP	CB-CG-OD2	5.06	122.85	118.30
2	D	201	ASP	CB-CG-OD2	5.05	122.85	118.30
2	B	156	ASP	CB-CG-OD2	5.05	122.84	118.30
2	A	122	ASP	CB-CG-OD2	5.05	122.84	118.30
2	E	259	ASP	CB-CG-OD2	5.04	122.83	118.30
2	C	411	ASP	CB-CG-OD2	5.03	122.83	118.30
2	F	411	ASP	CB-CG-OD2	5.03	122.83	118.30
2	D	328	ASP	CB-CG-OD2	5.03	122.83	118.30
2	C	48	ASP	CB-CG-OD2	5.02	122.82	118.30
2	B	201	ASP	CB-CG-OD2	5.02	122.82	118.30
2	B	290	ASP	CB-CG-OD2	5.02	122.82	118.30
2	F	290	ASP	CB-CG-OD2	5.02	122.82	118.30
2	D	52	ASP	CB-CG-OD2	5.02	122.81	118.30
2	D	411	ASP	CB-CG-OD2	5.01	122.81	118.30
2	C	156	ASP	CB-CG-OD2	5.00	122.80	118.30
2	D	233	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	355	PHE	Peptide
2	B	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	1	0
1	K	40	0	22	1	0
1	L	40	0	22	2	0
1	M	39	0	19	0	0
2	A	3210	0	3287	77	0
2	B	3213	0	3288	75	0
2	C	3213	0	3289	56	0
2	D	3213	0	3288	44	0
2	E	3206	0	3280	76	0
2	F	3213	0	3289	51	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	6	0
4	B	31	0	12	9	0
4	C	31	0	12	6	0
4	D	31	0	12	9	0
4	E	31	0	12	4	0
4	F	31	0	12	7	0
5	B	23	0	16	4	0
5	C	23	0	16	8	0
5	D	23	0	16	5	0
5	E	23	0	16	8	0
5	F	23	0	16	6	0
All	All	19814	0	20002	383	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 10.

All (383) 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	2.12	1.21
2:A:355:PHE:CE1	4:A:1600:AGS:H1'	1.82	1.12
2:C:366:ARG:HD2	4:D:4600:AGS:S1G	1.95	1.04
2:B:355:PHE:CZ	4:B:2600:AGS:H1'	1.94	1.03
2:C:140:HIS:HB3	2:C:306:ASN:HB3	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:355:PHE:HB3	2:C:356:PRO:HD2	1.39	1.00
2:A:167:PRO:CD	2:A:365:THR:HG21	1.91	0.99
2:A:167:PRO:HD2	2:A:365:THR:CG2	1.94	0.98
2:B:385:LYS:HA	2:B:388:HIS:CD2	1.98	0.98
2:A:167:PRO:HD2	2:A:365:THR:HG21	0.97	0.93
2:D:355:PHE:CD1	4:D:4600:AGS:H1'	2.05	0.91
2:A:355:PHE:CE1	4:A:1600:AGS:C1'	2.54	0.90
2:C:355:PHE:CB	2:C:356:PRO:HD2	2.04	0.86
2:C:183:GLY:HA2	4:C:3600:AGS:H8	1.58	0.84
2:F:183:GLY:HA2	4:F:6600:AGS:H8	1.62	0.81
2:F:183:GLY:CA	4:F:6600:AGS:H8	2.11	0.80
2:E:336:LYS:NZ	5:F:6701:FB:O12	2.13	0.80
2:F:141:ALA:HB1	2:F:370:LEU:HB2	1.64	0.80
2:A:139:LEU:O	2:A:306:ASN:ND2	2.15	0.79
2:A:355:PHE:CZ	4:A:1600:AGS:H1'	2.16	0.79
2:E:346:SER:HB3	2:E:349:ILE:HG22	1.66	0.78
2:D:355:PHE:HD1	4:D:4600:AGS:H1'	1.46	0.78
2:C:366:ARG:CD	4:D:4600:AGS:S1G	2.71	0.77
2:A:289:VAL:HG22	2:A:327:MET:HG3	1.67	0.77
2:B:132:LEU:HD22	2:B:251:LYS:HD2	1.66	0.77
2:E:340:ASN:HA	2:E:366:ARG:HD2	1.65	0.76
2:A:340:ASN:HA	2:A:366:ARG:HD2	1.68	0.76
2:F:349:ILE:HG22	2:F:354:VAL:HB	1.67	0.75
2:B:355:PHE:CZ	4:B:2600:AGS:C1'	2.71	0.74
2:B:355:PHE:CE1	4:B:2600:AGS:C1'	2.70	0.74
2:C:184:LYS:HD2	2:C:318:THR:HG21	1.72	0.72
2:D:341:MET:HG2	2:D:365:THR:HG22	1.70	0.72
2:A:172:GLN:H	2:A:314:THR:HB	1.55	0.71
2:A:365:THR:HG23	2:A:368:GLU:HG2	1.71	0.71
2:D:340:ASN:HA	2:D:366:ARG:HD2	1.71	0.71
2:B:385:LYS:HA	2:B:388:HIS:HD2	1.52	0.70
2:E:366:ARG:NE	4:F:6600:AGS:S1G	2.64	0.70
2:D:336:LYS:NZ	5:E:5701:FB:O12	2.22	0.70
2:F:140:HIS:O	2:F:141:ALA:HB2	1.90	0.69
2:B:185:THR:O	2:B:189:GLN:HB2	1.93	0.68
2:B:355:PHE:CE1	4:B:2600:AGS:O4'	2.48	0.67
2:A:289:VAL:CG2	2:A:327:MET:HG3	2.24	0.67
2:A:277:VAL:O	2:A:278:VAL:HG23	1.95	0.67
2:C:266:SER:H	2:C:318:THR:HB	1.61	0.66
2:E:212:ARG:H	2:E:212:ARG:HD2	1.59	0.66
2:F:141:ALA:CB	2:F:370:LEU:HB2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ASN:HB3	2:B:129:ASN:HD21	1.61	0.66
2:B:343:LEU:HD21	2:B:358:ILE:HG12	1.78	0.66
2:C:181:LYS:HG2	4:C:3600:AGS:S1G	2.37	0.65
2:E:7:LYS:HG2	2:E:35:ILE:HD13	1.78	0.65
2:D:138:PRO:HD2	2:D:306:ASN:O	1.97	0.64
2:E:355:PHE:CZ	4:E:5600:AGS:H1'	2.32	0.64
1:L:1:U:H2'	1:L:1:U:O2	1.98	0.63
2:E:169:GLY:H	2:E:172:GLN:HG3	1.63	0.63
2:C:355:PHE:HB3	2:C:356:PRO:CD	2.24	0.63
2:C:355:PHE:CB	2:C:356:PRO:CD	2.77	0.63
2:A:183:GLY:HA2	4:A:1600:AGS:H8	1.79	0.63
2:E:211:GLU:HA	5:E:5701:FB:C2B	2.29	0.62
2:B:2:ASN:ND2	2:B:50:PHE:HB2	2.14	0.62
2:B:355:PHE:CE1	4:B:2600:AGS:H1'	2.32	0.62
2:B:355:PHE:CE2	4:B:2600:AGS:H1'	2.35	0.61
2:C:130:LYS:HE3	2:D:11:VAL:HB	1.82	0.61
2:D:211:GLU:HA	5:D:4701:FB:C2B	2.30	0.61
2:E:187:LEU:O	2:E:191:ILE:HG12	2.01	0.61
2:B:388:HIS:HB2	2:B:389:PRO:HD3	1.82	0.61
2:F:23:LEU:HD22	2:F:26:LEU:HD23	1.82	0.61
2:E:238:ARG:HH12	2:E:242:VAL:HG13	1.66	0.60
2:F:211:GLU:HA	5:F:6701:FB:C2B	2.31	0.60
2:A:102:ARG:HB3	2:A:114:LEU:HD12	1.84	0.60
2:A:236:ALA:HA	2:A:239:HIS:HD2	1.66	0.60
2:B:154:THR:HA	2:B:157:LEU:HB2	1.83	0.60
2:A:166:SER:HA	2:A:365:THR:CG2	2.33	0.59
2:F:7:LYS:HG2	2:F:35:ILE:HD13	1.85	0.59
2:C:387:ILE:HG23	2:C:395:ALA:HB1	1.85	0.59
2:E:140:HIS:HA	2:E:306:ASN:HB2	1.84	0.58
2:E:178:ALA:HB2	2:E:345:LEU:HD12	1.84	0.58
2:F:140:HIS:O	2:F:141:ALA:CB	2.50	0.58
2:A:277:VAL:O	2:A:277:VAL:HG12	2.02	0.58
2:F:321:ILE:HG13	2:F:322:ASP:H	1.69	0.58
2:D:174:GLY:HA2	2:D:341:MET:HB3	1.86	0.57
2:D:355:PHE:CE1	4:D:4600:AGS:H1'	2.39	0.57
2:F:355:PHE:CD1	4:F:6600:AGS:N3	2.72	0.57
2:F:268:THR:HA	2:F:331:ILE:HG21	1.85	0.57
2:C:140:HIS:CD2	2:C:305:ARG:HB2	2.38	0.57
2:D:183:GLY:HA2	4:D:4600:AGS:H8	1.86	0.57
2:D:366:ARG:NE	4:E:5600:AGS:S1G	2.75	0.57
2:C:183:GLY:CA	4:C:3600:AGS:H8	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:GLY:HA3	5:C:3701:FB:H32	1.87	0.57
2:E:297:PRO:HB2	2:E:335:PHE:HZ	1.70	0.57
2:B:365:THR:HG23	2:B:368:GLU:HB3	1.86	0.56
2:C:388:HIS:HB3	2:C:389:PRO:HD3	1.86	0.56
5:C:3701:FB:H32	5:C:3701:FB:C7	2.36	0.56
2:D:183:GLY:CA	4:D:4600:AGS:H8	2.36	0.56
2:E:49:ILE:HG22	2:E:101:ILE:HG13	1.86	0.56
2:C:275:ASN:HD21	2:C:290:ASP:H	1.54	0.56
2:F:183:GLY:HA3	4:F:6600:AGS:H8	1.85	0.56
2:A:156:ASP:O	2:A:160:ARG:HB2	2.06	0.56
2:B:34:ILE:O	2:B:38:ILE:HG12	2.05	0.56
5:B:2701:FB:H32	5:B:2701:FB:C7	2.35	0.56
5:F:6701:FB:H32	5:F:6701:FB:C7	2.35	0.56
2:F:51:GLY:HA3	2:F:101:ILE:HD11	1.87	0.55
2:B:341:MET:HG2	2:B:365:THR:HB	1.89	0.55
2:C:379:LYS:HE2	2:C:412:PHE:HB2	1.87	0.55
2:D:49:ILE:HD13	2:D:49:ILE:H	1.71	0.55
2:A:372:THR:HB	2:A:376:GLU:HB3	1.88	0.55
2:E:337:GLY:O	5:F:6701:FB:H31	2.06	0.54
2:A:166:SER:HA	2:A:365:THR:HG21	1.88	0.54
2:A:355:PHE:HE1	4:A:1600:AGS:C1'	2.19	0.54
2:A:154:THR:HA	2:A:157:LEU:HD13	1.89	0.54
2:B:3:LEU:HD21	2:B:39:LEU:HD11	1.88	0.54
2:A:130:LYS:HZ1	2:A:309:GLU:HG2	1.73	0.54
2:A:369:GLU:HA	2:A:377:LEU:HD22	1.90	0.54
2:B:137:THR:HG22	2:B:305:ARG:HD3	1.90	0.54
2:B:366:ARG:CZ	4:C:3600:AGS:S1G	2.94	0.54
2:C:406:THR:HB	2:C:410:ASP:HB2	1.90	0.54
2:E:211:GLU:CD	5:E:5701:FB:HB1	2.29	0.54
2:E:141:ALA:HB1	2:E:370:LEU:HB2	1.90	0.53
2:B:209:ILE:HG13	2:B:270:LEU:HB2	1.90	0.53
2:A:280:ALA:C	2:A:284:VAL:N	2.62	0.53
2:C:290:ASP:HB3	2:C:293:ALA:HB2	1.91	0.53
2:D:275:ASN:HA	2:D:293:ALA:HB1	1.90	0.53
2:A:279:PRO:HA	2:A:290:ASP:OD2	2.08	0.53
2:E:403:LEU:HA	2:E:411:ASP:OD2	2.08	0.53
2:B:2:ASN:ND2	2:B:50:PHE:HD2	2.07	0.53
2:F:358:ILE:O	2:F:359:ASP:CB	2.57	0.53
2:D:132:LEU:HD13	2:D:251:LYS:HA	1.91	0.52
2:F:248:GLU:O	2:F:252:ARG:HG2	2.08	0.52
2:F:355:PHE:HB2	2:F:356:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:ARG:HA	2:C:233:ASP:HB2	1.92	0.52
2:E:176:ILE:HB	2:E:318:THR:HG22	1.92	0.52
5:E:5701:FB:C7	5:E:5701:FB:H32	2.39	0.52
2:B:143:SER:HB2	2:B:170:ARG:HD3	1.90	0.52
2:C:387:ILE:HD11	2:C:399:LEU:HD13	1.91	0.52
5:D:4701:FB:C7	5:D:4701:FB:H32	2.37	0.52
2:D:269:ARG:HD3	2:D:272:ARG:HD2	1.90	0.52
2:E:337:GLY:HA3	5:F:6701:FB:C3	2.40	0.52
2:F:347:ARG:HA	2:F:350:ALA:HB3	1.92	0.52
5:B:2701:FB:C7	5:B:2701:FB:C3	2.88	0.52
2:A:279:PRO:O	2:A:280:ALA:CB	2.57	0.52
2:B:332:TYR:O	2:B:336:LYS:HG3	2.10	0.52
2:C:174:GLY:HA2	2:C:341:MET:HB3	1.92	0.52
2:E:265:ASP:OD1	5:E:5701:FB:HA2	2.09	0.52
2:E:352:LYS:O	2:E:354:VAL:N	2.42	0.52
2:B:145:LEU:HG	2:B:170:ARG:HD2	1.92	0.51
2:D:139:LEU:HD22	2:D:367:LYS:HG3	1.91	0.51
5:C:3701:FB:C7	5:C:3701:FB:C3	2.87	0.51
2:F:327:MET:O	2:F:331:ILE:HG12	2.10	0.51
2:E:147:MET:HG3	2:E:162:LEU:HD23	1.92	0.51
2:D:132:LEU:HD22	2:D:251:LYS:HG2	1.92	0.51
2:A:131:ILE:HD12	2:A:133:PHE:HD2	1.76	0.50
2:C:144:ARG:NH2	2:C:167:PRO:HB3	2.26	0.50
2:A:56:GLU:HA	2:A:93:THR:HG23	1.93	0.50
2:D:268:THR:HG21	2:D:320:LEU:H	1.75	0.50
2:F:388:HIS:HB3	2:F:389:PRO:HD3	1.94	0.50
2:D:284:VAL:HG23	2:D:285:LEU:HD12	1.94	0.50
2:E:98:SER:HB2	2:E:118:GLU:HB2	1.93	0.50
2:F:160:ARG:HG3	2:F:408:THR:HB	1.92	0.50
2:C:140:HIS:CG	2:C:306:ASN:H	2.29	0.50
2:C:348:LYS:HG2	2:C:393:ILE:HD11	1.92	0.50
2:A:65:LEU:HD11	2:A:97:ILE:HB	1.94	0.50
2:B:3:LEU:HD13	2:B:79:ILE:HD11	1.93	0.50
2:F:355:PHE:CD1	4:F:6600:AGS:H1'	2.47	0.50
2:A:140:HIS:ND1	2:A:340:ASN:ND2	2.59	0.49
2:A:279:PRO:O	2:A:280:ALA:HB2	2.12	0.49
2:E:140:HIS:HB3	2:E:306:ASN:HB2	1.94	0.49
2:B:65:LEU:HB2	2:B:79:ILE:HB	1.93	0.49
2:E:31:LYS:HA	2:E:34:ILE:HD12	1.95	0.49
5:D:4701:FB:C7	5:D:4701:FB:C3	2.89	0.49
2:E:140:HIS:CA	2:E:306:ASN:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ASP:OD1	2:B:53:GLY:N	2.46	0.49
2:A:13:GLU:O	2:A:16:THR:HG23	2.13	0.49
2:C:183:GLY:HA2	4:C:3600:AGS:C8	2.36	0.49
2:B:30:ARG:O	2:B:34:ILE:HG12	2.12	0.49
2:C:160:ARG:HD2	2:C:403:LEU:HD12	1.93	0.49
2:C:211:GLU:HA	5:C:3701:FB:C2B	2.43	0.49
2:C:294:LEU:HD21	2:C:331:ILE:HG12	1.95	0.49
2:D:147:MET:HE1	2:D:191:ILE:HG12	1.94	0.48
2:E:140:HIS:CB	2:E:306:ASN:HB2	2.43	0.48
2:A:355:PHE:CB	2:A:356:PRO:CD	2.90	0.48
2:B:236:ALA:HA	2:B:239:HIS:HD2	1.77	0.48
2:B:386:ILE:HG23	2:B:387:ILE:HD12	1.94	0.48
2:C:184:LYS:HD2	2:C:318:THR:CG2	2.40	0.48
2:D:140:HIS:ND1	2:D:140:HIS:O	2.46	0.48
2:A:268:THR:O	2:A:272:ARG:HG3	2.13	0.48
2:A:289:VAL:HG22	2:A:327:MET:CG	2.42	0.48
2:B:2:ASN:ND2	2:B:50:PHE:CD2	2.82	0.48
2:E:144:ARG:HA	2:E:169:GLY:HA2	1.95	0.48
2:F:2:ASN:HA	2:F:50:PHE:HB2	1.95	0.48
1:L:1:U:H1'	2:F:110:TYR:HE2	1.79	0.48
2:D:294:LEU:HD21	2:D:331:ILE:HG12	1.96	0.48
2:E:408:THR:O	2:E:409:ASN:HB2	2.14	0.48
2:D:345:LEU:HA	2:D:357:ALA:O	2.13	0.48
2:E:352:LYS:HE2	2:E:353:ARG:N	2.29	0.48
2:A:176:ILE:HB	2:A:318:THR:HG22	1.96	0.48
2:B:2:ASN:HD22	2:B:50:PHE:HD2	1.59	0.48
2:C:31:LYS:O	2:C:35:ILE:HG12	2.14	0.48
2:E:238:ARG:NH1	2:E:242:VAL:HG13	2.28	0.48
2:F:30:ARG:O	2:F:34:ILE:HG12	2.14	0.48
2:A:3:LEU:HD23	2:A:39:LEU:HD23	1.96	0.48
2:B:337:GLY:HA3	5:C:3701:FB:C3	2.43	0.48
2:B:356:PRO:C	2:B:358:ILE:H	2.17	0.48
2:C:337:GLY:O	5:D:4701:FB:H31	2.14	0.48
2:D:212:ARG:NH2	4:D:4600:AGS:S1G	2.87	0.48
2:D:296:ARG:HB2	2:D:297:PRO:HD3	1.96	0.48
2:C:144:ARG:HD2	2:C:371:LEU:O	2.14	0.47
2:E:209:ILE:HD13	2:E:270:LEU:HD13	1.96	0.47
2:E:381:TRP:HA	2:E:381:TRP:CE3	2.49	0.47
2:F:3:LEU:HA	2:F:6:LEU:HD12	1.96	0.47
2:E:34:ILE:O	2:E:38:ILE:HG12	2.14	0.47
2:E:323:THR:HG23	5:E:5701:FB:O12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:72:TYR:HB3	2:F:245:MET:HE3	1.96	0.47
5:F:6701:FB:C7	5:F:6701:FB:C3	2.87	0.47
2:E:321:ILE:HG13	2:E:322:ASP:H	1.79	0.47
5:E:5701:FB:C7	5:E:5701:FB:C3	2.91	0.47
2:A:250:ALA:O	2:A:254:VAL:HG23	2.15	0.47
2:C:18:GLY:HA3	2:C:26:LEU:CD1	2.45	0.47
1:J:1:U:H1'	2:D:110:TYR:CE2	2.49	0.46
2:B:296:ARG:HB2	2:B:297:PRO:HD3	1.97	0.46
2:D:349:ILE:HD11	2:D:392:GLU:HG2	1.96	0.46
2:D:396:MET:O	2:D:400:ILE:HG12	2.15	0.46
2:A:144:ARG:HH12	2:A:372:THR:HG22	1.81	0.46
2:B:156:ASP:O	2:B:160:ARG:HG2	2.15	0.46
2:E:138:PRO:HD2	2:E:306:ASN:O	2.15	0.46
2:E:254:VAL:HG21	2:E:313:LEU:HB2	1.96	0.46
2:E:275:ASN:HA	2:E:293:ALA:HB1	1.97	0.46
2:A:4:THR:HG22	2:A:7:LYS:HD3	1.97	0.46
2:E:158:THR:HG21	4:E:5600:AGS:HN62	1.80	0.46
2:F:157:LEU:O	2:F:161:VAL:HG23	2.15	0.46
2:A:178:ALA:HB3	2:A:184:LYS:HD3	1.98	0.46
2:B:211:GLU:HA	5:B:2701:FB:C2B	2.46	0.46
2:B:384:ARG:HB3	2:B:388:HIS:CE1	2.51	0.46
2:F:207:LEU:HD13	2:F:246:VAL:HG21	1.98	0.46
2:B:57:ILE:H	2:B:93:THR:HB	1.81	0.46
2:B:137:THR:O	2:C:214:GLU:HA	2.16	0.46
2:B:340:ASN:HA	2:B:366:ARG:NH1	2.31	0.46
2:A:53:GLY:HA3	2:A:65:LEU:HB3	1.98	0.46
2:C:306:ASN:CG	2:C:306:ASN:O	2.54	0.46
2:F:207:LEU:HD11	2:F:242:VAL:HG12	1.97	0.46
2:B:175:LEU:O	2:B:342:GLU:HA	2.15	0.45
2:B:177:VAL:HG13	2:B:321:ILE:HG13	1.98	0.45
2:D:268:THR:HA	2:D:331:ILE:HG21	1.98	0.45
2:E:172:GLN:H	2:E:314:THR:HB	1.82	0.45
2:D:173:ARG:NH2	2:E:214:GLU:OE1	2.49	0.45
2:F:34:ILE:O	2:F:38:ILE:HG12	2.16	0.45
2:F:279:PRO:HB2	2:F:280:ALA:H	1.60	0.45
2:A:143:SER:HB2	2:A:170:ARG:HE	1.81	0.45
2:A:261:ILE:HG12	2:A:314:THR:HG23	1.97	0.45
2:B:183:GLY:HA2	4:B:2600:AGS:H8	1.98	0.45
2:D:240:VAL:HG21	2:D:277:VAL:HG11	1.97	0.45
2:F:174:GLY:HA3	2:F:316:ILE:HG13	1.98	0.45
2:E:211:GLU:OE1	5:E:5701:FB:HB1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:GLY:HA3	4:F:6600:AGS:C8	2.46	0.45
2:A:278:VAL:HA	2:A:279:PRO:HD3	1.58	0.45
2:E:261:ILE:HG12	2:E:314:THR:HG23	1.99	0.45
2:F:173:ARG:HD3	2:F:302:GLY:HA2	1.99	0.45
2:C:211:GLU:O	2:C:231:THR:HA	2.16	0.45
2:E:211:GLU:O	2:E:231:THR:HA	2.17	0.45
2:F:187:LEU:O	2:F:191:ILE:HG12	2.17	0.45
2:B:254:VAL:HG21	2:B:313:LEU:HB2	1.99	0.44
2:F:39:LEU:HB3	2:F:111:PHE:CZ	2.52	0.44
2:A:166:SER:HB2	2:A:365:THR:HB	1.98	0.44
2:A:174:GLY:HA2	2:A:341:MET:HB3	1.99	0.44
2:A:352:LYS:O	2:A:354:VAL:HG23	2.18	0.44
2:B:355:PHE:CG	4:B:2600:AGS:C4	3.01	0.44
2:A:183:GLY:CA	4:A:1600:AGS:H8	2.45	0.44
2:B:1:MET:O	2:B:49:ILE:HA	2.17	0.44
2:C:207:LEU:HD13	2:C:246:VAL:HG21	1.98	0.44
2:E:251:LYS:O	2:E:255:GLU:HG3	2.18	0.44
2:A:17:LEU:HB3	2:A:21:MET:HG3	2.00	0.44
2:C:178:ALA:HB2	2:C:345:LEU:HD12	1.99	0.44
2:A:355:PHE:CB	2:A:356:PRO:HD2	2.48	0.44
2:A:355:PHE:HB3	2:A:356:PRO:CD	2.47	0.44
2:B:336:LYS:NZ	5:C:3701:FB:O12	2.50	0.44
2:E:132:LEU:HD13	2:E:251:LYS:HA	2.00	0.44
2:F:349:ILE:HB	2:F:357:ALA:HB1	1.99	0.44
2:A:173:ARG:HG3	2:A:304:ALA:HB3	2.00	0.44
2:B:131:ILE:HD12	2:B:133:PHE:HB2	2.00	0.43
2:C:138:PRO:HD2	2:C:140:HIS:CE1	2.53	0.43
2:F:138:PRO:HD2	2:F:306:ASN:O	2.18	0.43
2:C:269:ARG:NH2	5:C:3701:FB:O7	2.49	0.43
2:F:167:PRO:HD2	2:F:365:THR:HG22	2.00	0.43
2:B:54:VAL:HG22	2:B:96:THR:HG22	2.00	0.43
2:B:171:GLY:H	2:B:314:THR:HB	1.84	0.43
2:A:11:VAL:HG22	2:A:31:LYS:HE3	2.01	0.43
2:A:171:GLY:HA3	2:A:312:SER:HB2	2.00	0.43
2:A:207:LEU:HD13	2:A:246:VAL:HG21	2.00	0.43
2:B:169:GLY:H	2:B:172:GLN:HG3	1.83	0.43
2:B:268:THR:HG21	2:B:320:LEU:HB2	1.99	0.43
2:E:158:THR:HA	2:E:356:PRO:HG3	1.99	0.43
2:E:173:ARG:HG3	2:E:304:ALA:HB3	2.01	0.43
2:B:3:LEU:HD22	2:B:7:LYS:HZ2	1.83	0.43
2:E:113:LEU:HD21	2:E:116:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:349:ILE:HG23	2:E:357:ALA:HB1	2.01	0.43
2:F:321:ILE:HG13	2:F:322:ASP:N	2.32	0.43
2:B:268:THR:HA	2:B:331:ILE:HG21	2.01	0.43
2:D:355:PHE:HB2	2:D:356:PRO:HD3	2.01	0.43
2:A:388:HIS:N	2:A:389:PRO:HD2	2.34	0.43
2:A:206:VAL:HG21	2:A:223:VAL:HG11	2.00	0.43
2:A:355:PHE:HB2	2:A:356:PRO:HD2	1.99	0.43
2:A:355:PHE:O	2:A:356:PRO:C	2.56	0.43
2:B:207:LEU:O	2:B:264:LEU:HA	2.19	0.43
2:E:6:LEU:HD22	2:E:35:ILE:HG23	2.01	0.43
2:B:170:ARG:HB3	2:B:312:SER:OG	2.18	0.42
2:D:355:PHE:HD1	4:D:4600:AGS:C1'	2.24	0.42
2:E:266:SER:HB3	2:E:269:ARG:HB2	2.01	0.42
2:A:129:ASN:HD22	2:A:129:ASN:HA	1.63	0.42
2:D:406:THR:HB	2:D:407:LYS:H	1.68	0.42
2:E:262:ILE:HB	2:E:315:ILE:HG12	2.00	0.42
2:C:137:THR:O	2:D:214:GLU:HA	2.20	0.42
2:D:290:ASP:HB3	2:D:293:ALA:HB2	2.01	0.42
2:E:309:GLU:H	2:E:309:GLU:HG2	1.62	0.42
2:B:138:PRO:HD2	2:B:306:ASN:O	2.19	0.42
2:C:137:THR:HA	2:C:140:HIS:CE1	2.54	0.42
2:D:268:THR:HG21	2:D:320:LEU:HB2	2.00	0.42
2:E:207:LEU:HA	2:E:228:VAL:O	2.19	0.42
2:E:355:PHE:CZ	4:E:5600:AGS:C1'	3.01	0.42
2:E:357:ALA:O	2:E:358:ILE:C	2.57	0.42
2:E:388:HIS:HB3	2:E:389:PRO:HD3	2.02	0.42
2:A:166:SER:CB	2:A:365:THR:HB	2.50	0.42
2:B:349:ILE:HG12	2:B:393:ILE:HG13	2.01	0.42
2:F:144:ARG:HA	2:F:169:GLY:HA2	2.01	0.42
2:F:349:ILE:HB	2:F:357:ALA:CB	2.50	0.42
2:F:406:THR:HB	2:F:407:LYS:H	1.57	0.42
1:K:2:C:H42	2:E:74:ALA:HB1	1.83	0.42
2:A:261:ILE:HG12	2:A:314:THR:CG2	2.50	0.42
2:F:39:LEU:HD11	2:F:49:ILE:HG21	2.02	0.42
2:A:202:CYS:HB3	2:A:259:ASP:HB2	2.02	0.42
2:B:257:LYS:HG2	2:B:310:GLY:HA3	2.02	0.42
2:B:355:PHE:CD2	4:B:2600:AGS:N3	2.87	0.42
2:B:162:LEU:HD11	2:B:187:LEU:HD21	2.02	0.42
2:B:207:LEU:HD13	2:B:246:VAL:HG21	2.02	0.42
2:B:266:SER:HB3	2:B:269:ARG:HB2	2.01	0.42
2:C:257:LYS:HG2	2:C:310:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:72:TYR:CG	2:F:245:MET:HG2	2.55	0.42
2:C:138:PRO:HD2	2:C:140:HIS:HE1	1.84	0.41
2:E:3:LEU:HB3	2:E:51:GLY:HA2	2.02	0.41
2:E:263:LEU:HD23	2:E:316:ILE:HB	2.01	0.41
2:F:358:ILE:O	2:F:359:ASP:HB2	2.19	0.41
2:A:140:HIS:CE1	2:A:340:ASN:OD1	2.73	0.41
2:A:337:GLY:O	5:B:2701:FB:H31	2.21	0.41
2:B:309:GLU:H	2:B:309:GLU:HG2	1.63	0.41
2:E:189:GLN:HE22	2:E:218:GLU:HG2	1.85	0.41
2:C:337:GLY:HA3	5:D:4701:FB:C3	2.50	0.41
2:D:160:ARG:HB3	2:D:408:THR:HG21	2.01	0.41
2:D:207:LEU:HD13	2:D:246:VAL:HG21	2.03	0.41
2:E:60:ASP:HB2	2:E:62:PHE:HE2	1.85	0.41
2:B:3:LEU:CD1	2:B:79:ILE:HD11	2.50	0.41
2:C:32:GLN:HB3	2:C:76:PRO:HD2	2.02	0.41
2:C:47:GLU:HB3	2:C:48:ASP:H	1.65	0.41
2:C:173:ARG:HD2	2:C:301:PHE:O	2.20	0.41
2:E:3:LEU:HD22	2:E:79:ILE:HD11	2.02	0.41
2:A:17:LEU:HB3	2:A:21:MET:CG	2.51	0.41
2:B:349:ILE:HG22	2:B:349:ILE:O	2.21	0.41
2:B:102:ARG:HA	2:B:103:PRO:HD3	1.93	0.41
2:E:141:ALA:CB	2:E:370:LEU:HB2	2.51	0.41
2:E:381:TRP:HA	2:E:381:TRP:HE3	1.85	0.41
2:A:147:MET:HE2	2:A:194:SER:HB3	2.03	0.41
2:A:365:THR:O	2:A:366:ARG:O	2.39	0.41
2:C:31:LYS:HA	2:C:34:ILE:HD12	2.03	0.41
2:C:382:ILE:O	2:C:386:ILE:HG12	2.20	0.41
2:A:277:VAL:O	2:A:277:VAL:CG1	2.69	0.41
2:B:337:GLY:O	5:C:3701:FB:H31	2.21	0.41
2:C:169:GLY:H	2:C:172:GLN:CG	2.34	0.41
2:E:294:LEU:C	2:E:297:PRO:HD2	2.42	0.41
2:E:168:ILE:HD11	2:E:341:MET:HE3	2.03	0.40
2:E:248:GLU:O	2:E:252:ARG:HG2	2.21	0.40
2:A:352:LYS:HE3	2:F:295:HIS:HE1	1.86	0.40
2:C:268:THR:HA	2:C:331:ILE:HG21	2.02	0.40
2:D:387:ILE:O	2:D:390:MET:HG2	2.21	0.40
2:E:171:GLY:H	2:E:314:THR:HB	1.86	0.40
2:E:173:ARG:HD3	2:E:302:GLY:HA2	2.03	0.40
2:E:379:LYS:HG3	2:E:412:PHE:CG	2.56	0.40
2:F:178:ALA:HB3	2:F:184:LYS:HD3	2.02	0.40
2:C:158:THR:HG23	2:C:356:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:ILE:HB	2:D:318:THR:HG22	2.02	0.40
2:A:352:LYS:O	2:A:354:VAL:N	2.54	0.40
2:D:144:ARG:HG3	2:D:146:ARG:H	1.85	0.40
2:A:191:ILE:HG21	2:A:263:LEU:HD21	2.03	0.40
2:A:374:GLN:H	2:A:374:GLN:HE21	1.69	0.40
2:A:385:LYS:NZ	2:B:353:ARG:HH21	2.20	0.40
2:C:169:GLY:O	2:C:172:GLN:HG2	2.21	0.40
2:E:268:THR:HA	2:E:331:ILE:HG21	2.04	0.40
2:F:254:VAL:HG21	2:F:313:LEU:HB2	2.03	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%)	356 (89%)	35 (9%)	9 (2%)	6 31
2	B	400/419 (96%)	362 (90%)	35 (9%)	3 (1%)	19 55
2	C	400/419 (96%)	372 (93%)	23 (6%)	5 (1%)	12 44
2	D	400/419 (96%)	374 (94%)	20 (5%)	6 (2%)	10 41
2	E	399/419 (95%)	367 (92%)	28 (7%)	4 (1%)	15 51
2	F	400/419 (96%)	368 (92%)	26 (6%)	6 (2%)	10 41
All	All	2399/2514 (95%)	2199 (92%)	167 (7%)	33 (1%)	11 43

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	353	ARG
2	A	355	PHE
2	A	356	PRO

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Mol	Chain	Res	Type
2	A	366	ARG
2	B	355	PHE
2	B	356	PRO
2	F	141	ALA
2	F	142	ASN
2	C	141	ALA
2	C	355	PHE
2	D	24	GLU
2	D	90	ASN
2	D	140	HIS
2	D	146	ARG
2	E	353	ARG
2	F	279	PRO
2	F	359	ASP
2	A	138	PRO
2	A	279	PRO
2	C	106	GLU
2	C	266	SER
2	D	407	LYS
2	E	358	ILE
2	F	266	SER
2	D	124	PRO
2	A	15	ILE
2	A	266	SER
2	E	266	SER
2	E	409	ASN
2	F	94	GLY
2	A	278	VAL
2	B	209	ILE
2	C	307	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
2	A	350/359 (98%)	329 (94%)	21 (6%)	19 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	351/359 (98%)	324 (92%)	27 (8%)	13	41
2	C	351/359 (98%)	334 (95%)	17 (5%)	25	59
2	D	351/359 (98%)	323 (92%)	28 (8%)	12	39
2	E	350/359 (98%)	327 (93%)	23 (7%)	16	47
2	F	351/359 (98%)	334 (95%)	17 (5%)	25	59
All	All	2104/2154 (98%)	1971 (94%)	133 (6%)	18	49

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	14	LEU
2	A	16	THR
2	A	48	ASP
2	A	52	ASP
2	A	65	LEU
2	A	123	LYS
2	A	155	GLU
2	A	194	SER
2	A	226	GLU
2	A	247	ILE
2	A	292	ASN
2	A	299	ARG
2	A	306	ASN
2	A	314	THR
2	A	341	MET
2	A	347	ARG
2	A	348	LYS
2	A	361	ASN
2	A	374	GLN
2	A	381	TRP
2	A	405	MET
2	B	14	LEU
2	B	26	LEU
2	B	60	ASP
2	B	91	LEU
2	B	93	THR
2	B	100	LYS
2	B	108	GLU
2	B	122	ASP
2	B	130	LYS

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Mol	Chain	Res	Type
2	B	132	LEU
2	B	139	LEU
2	B	157	LEU
2	B	172	GLN
2	B	187	LEU
2	B	218	GLU
2	B	244	GLU
2	B	252	ARG
2	B	268	THR
2	B	299	ARG
2	B	314	THR
2	B	331	ILE
2	B	333	GLU
2	B	340	ASN
2	B	383	LEU
2	B	387	ILE
2	B	409	ASN
2	B	411	ASP
2	C	19	GLU
2	C	49	ILE
2	C	93	THR
2	C	125	GLU
2	C	137	THR
2	C	139	LEU
2	C	160	ARG
2	C	186	MET
2	C	187	LEU
2	C	188	LEU
2	C	193	GLN
2	C	284	VAL
2	C	306	ASN
2	C	314	THR
2	C	354	VAL
2	C	383	LEU
2	C	394	ASP
2	D	4	THR
2	D	14	LEU
2	D	49	ILE
2	D	69	ASP
2	D	89	PHE
2	D	100	LYS
2	D	110	TYR

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Mol	Chain	Res	Type
2	D	115	LYS
2	D	129	ASN
2	D	130	LYS
2	D	136	LEU
2	D	139	LEU
2	D	170	ARG
2	D	184	LYS
2	D	190	ASN
2	D	212	ARG
2	D	222	LEU
2	D	244	GLU
2	D	252	ARG
2	D	286	THR
2	D	309	GLU
2	D	314	THR
2	D	327	MET
2	D	362	ARG
2	D	378	GLN
2	D	399	LEU
2	D	403	LEU
2	D	413	PHE
2	E	6	LEU
2	E	8	ASN
2	E	9	THR
2	E	77	ASP
2	E	93	THR
2	E	155	GLU
2	E	158	THR
2	E	212	ARG
2	E	242	VAL
2	E	245	MET
2	E	266	SER
2	E	267	ILE
2	E	285	LEU
2	E	290	ASP
2	E	314	THR
2	E	322	ASP
2	E	347	ARG
2	E	352	LYS
2	E	353	ARG
2	E	361	ASN
2	E	369	GLU

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Mol	Chain	Res	Type
2	E	381	TRP
2	E	406	THR
2	F	9	THR
2	F	93	THR
2	F	96	THR
2	F	97	ILE
2	F	105	LYS
2	F	122	ASP
2	F	133	PHE
2	F	134	GLU
2	F	160	ARG
2	F	162	LEU
2	F	193	GLN
2	F	226	GLU
2	F	241	GLN
2	F	340	ASN
2	F	399	LEU
2	F	406	THR
2	F	412	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	59	GLN
2	A	129	ASN
2	A	135	ASN
2	A	193	GLN
2	A	256	HIS
2	A	275	ASN
2	A	374	GLN
2	B	126	ASN
2	B	129	ASN
2	B	172	GLN
2	B	256	HIS
2	B	275	ASN
2	B	306	ASN
2	B	388	HIS
2	C	20	ASN
2	C	41	GLN
2	C	90	ASN
2	C	117	ASN
2	C	120	ASN

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Mol	Chain	Res	Type
2	C	275	ASN
2	D	90	ASN
2	D	198	ASN
2	D	275	ASN
2	D	292	ASN
2	D	306	ASN
2	E	41	GLN
2	E	189	GLN
2	E	361	ASN
2	F	90	ASN
2	F	189	GLN
2	F	241	GLN
2	F	295	HIS
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%)	1 (100%)	0
1	L	1/8 (12%)	1 (100%)	0
1	M	1/8 (12%)	0	1 (100%)
All	All	6/48 (12%)	5 (83%)	1 (16%)

All (5) RNA backbone outliers are listed below:

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

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	M	1	U

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	$\#\|Z\| > 2$
4	AGS	B	2600	3	26,33,33	2.32	5 (19%)	26,52,52	1.58	7 (26%)
5	FB	D	4701	-	17,24,24	2.72	4 (23%)	12,38,38	9.27	3 (25%)
5	FB	E	5701	-	17,24,24	2.51	4 (23%)	12,38,38	5.73	3 (25%)
5	FB	F	6701	-	17,24,24	2.60	4 (23%)	12,38,38	6.13	4 (33%)
4	AGS	E	5600	3	26,33,33	2.26	5 (19%)	26,52,52	1.55	6 (23%)
4	AGS	F	6600	3	26,33,33	2.24	4 (15%)	26,52,52	1.59	5 (19%)
4	AGS	C	3600	3	26,33,33	2.21	4 (15%)	26,52,52	1.59	6 (23%)
4	AGS	D	4600	3	26,33,33	2.24	4 (15%)	26,52,52	1.57	5 (19%)
5	FB	C	3701	-	17,24,24	2.69	4 (23%)	12,38,38	8.29	3 (25%)
4	AGS	A	1600	3	26,33,33	2.34	4 (15%)	26,52,52	1.53	6 (23%)
5	FB	B	2701	-	17,24,24	2.80	4 (23%)	12,38,38	6.56	3 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	B	2600	3	-	3/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FB	D	4701	-	-	7/10/53/53	0/1/2/2
5	FB	E	5701	-	-	10/10/53/53	0/1/2/2
5	FB	F	6701	-	-	7/10/53/53	0/1/2/2
4	AGS	E	5600	3	-	4/17/38/38	0/3/3/3
4	AGS	F	6600	3	-	5/17/38/38	0/3/3/3
4	AGS	C	3600	3	-	5/17/38/38	0/3/3/3
4	AGS	D	4600	3	-	5/17/38/38	0/3/3/3
5	FB	C	3701	-	-	7/10/53/53	0/1/2/2
4	AGS	A	1600	3	-	4/17/38/38	0/3/3/3
5	FB	B	2701	-	-	7/10/53/53	0/1/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2701	FB	C5A-C12	-8.38	1.24	1.44
5	D	4701	FB	C5A-C12	-8.24	1.25	1.44
5	C	3701	FB	C5A-C12	-7.80	1.26	1.44
4	A	1600	AGS	PG-S1G	7.70	2.07	1.90
4	B	2600	AGS	PG-S1G	7.50	2.07	1.90
5	F	6701	FB	C5A-C12	-7.35	1.27	1.44
4	E	5600	AGS	PG-S1G	7.22	2.06	1.90
4	D	4600	AGS	PG-S1G	7.18	2.06	1.90
4	F	6600	AGS	PG-S1G	7.15	2.06	1.90
5	E	5701	FB	C5A-C12	-6.94	1.28	1.44
4	C	3600	AGS	PG-S1G	6.90	2.05	1.90
4	A	1600	AGS	C4-N3	6.70	1.44	1.35
4	B	2600	AGS	C4-N3	6.61	1.44	1.35
4	E	5600	AGS	C4-N3	6.56	1.44	1.35
4	D	4600	AGS	C4-N3	6.52	1.44	1.35
4	F	6600	AGS	C4-N3	6.49	1.44	1.35
4	C	3600	AGS	C4-N3	6.46	1.44	1.35
5	B	2701	FB	C5A-C5	-5.86	1.26	1.33
5	E	5701	FB	C5A-C5	-5.34	1.26	1.33
5	F	6701	FB	C5A-C5	-5.32	1.26	1.33
5	C	3701	FB	C5A-C5	-5.24	1.27	1.33
5	D	4701	FB	C5A-C5	-5.13	1.27	1.33
5	C	3701	FB	O6-C6	4.23	1.44	1.40
5	F	6701	FB	O6-C6	4.10	1.44	1.40
5	D	4701	FB	O6-C6	3.63	1.44	1.40
5	B	2701	FB	O6-C6	3.42	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	5701	FB	O6-C6	3.34	1.43	1.40
5	D	4701	FB	C4-C5	2.71	1.54	1.50
5	C	3701	FB	C4-C5	2.58	1.54	1.50
4	E	5600	AGS	PA-O1A	2.54	1.59	1.50
4	A	1600	AGS	PA-O1A	2.54	1.59	1.50
4	D	4600	AGS	PA-O1A	2.54	1.59	1.50
4	F	6600	AGS	PA-O1A	2.53	1.59	1.50
4	C	3600	AGS	PA-O1A	2.52	1.59	1.50
4	B	2600	AGS	PA-O1A	2.51	1.59	1.50
5	E	5701	FB	C4-C5	2.48	1.54	1.50
5	F	6701	FB	C4-C5	2.48	1.54	1.50
4	B	2600	AGS	PB-O1B	2.41	1.59	1.50
4	A	1600	AGS	PB-O1B	2.40	1.59	1.50
5	B	2701	FB	C4-C5	2.39	1.54	1.50
4	F	6600	AGS	PB-O1B	2.38	1.59	1.50
4	E	5600	AGS	PB-O1B	2.37	1.59	1.50
4	D	4600	AGS	PB-O1B	2.34	1.59	1.50
4	C	3600	AGS	PB-O1B	2.31	1.59	1.50
4	B	2600	AGS	O4'-C1'	2.14	1.44	1.41
4	E	5600	AGS	O4'-C1'	2.00	1.43	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	4701	FB	O12-C12-C5A	31.21	161.64	123.66
5	C	3701	FB	O12-C12-C5A	27.73	157.41	123.66
5	B	2701	FB	O12-C12-C5A	21.44	149.76	123.66
5	F	6701	FB	O12-C12-C5A	19.75	147.69	123.66
5	E	5701	FB	O12-C12-C5A	18.28	145.91	123.66
5	F	6701	FB	C7-C6-N10	6.74	118.50	109.66
5	E	5701	FB	C7-C6-N10	6.60	118.32	109.66
5	B	2701	FB	C7-C6-N10	6.49	118.17	109.66
5	D	4701	FB	C7-C6-N10	6.45	118.12	109.66
5	C	3701	FB	C7-C6-N10	6.43	118.09	109.66
4	F	6600	AGS	N3-C2-N1	-3.84	122.68	128.68
4	D	4600	AGS	N3-C2-N1	-3.83	122.70	128.68
4	A	1600	AGS	N3-C2-N1	-3.81	122.72	128.68
4	E	5600	AGS	N3-C2-N1	-3.80	122.75	128.68
4	B	2600	AGS	N3-C2-N1	-3.79	122.75	128.68
4	C	3600	AGS	N3-C2-N1	-3.61	123.03	128.68
4	C	3600	AGS	C3'-C2'-C1'	3.51	106.27	100.98
4	F	6600	AGS	C3'-C2'-C1'	3.29	105.94	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2600	AGS	C4-C5-N7	-3.21	106.05	109.40
4	D	4600	AGS	C3'-C2'-C1'	3.20	105.80	100.98
4	E	5600	AGS	C3'-C2'-C1'	3.19	105.78	100.98
4	C	3600	AGS	C4-C5-N7	-3.19	106.08	109.40
4	F	6600	AGS	C4-C5-N7	-3.18	106.09	109.40
4	D	4600	AGS	C4-C5-N7	-3.13	106.14	109.40
4	E	5600	AGS	C4-C5-N7	-3.06	106.21	109.40
4	A	1600	AGS	C4-C5-N7	-3.05	106.22	109.40
5	E	5701	FB	O2A-C2A-C1A	2.82	112.56	107.63
4	A	1600	AGS	C3'-C2'-C1'	2.77	105.15	100.98
5	F	6701	FB	O2A-C2A-C1A	2.73	112.42	107.63
5	D	4701	FB	O2A-C2A-C1A	2.73	112.41	107.63
4	B	2600	AGS	C3'-C2'-C1'	2.69	105.02	100.98
5	B	2701	FB	O2A-C2A-C1A	2.64	112.26	107.63
4	E	5600	AGS	C2-N1-C6	2.57	123.14	118.75
4	A	1600	AGS	C2-N1-C6	2.56	123.13	118.75
4	D	4600	AGS	C2-N1-C6	2.54	123.10	118.75
4	B	2600	AGS	C2-N1-C6	2.53	123.08	118.75
4	C	3600	AGS	C2-N1-C6	2.52	123.07	118.75
5	C	3701	FB	O2A-C2A-C1A	2.52	112.06	107.63
4	F	6600	AGS	C2-N1-C6	2.50	123.03	118.75
4	B	2600	AGS	C2'-C3'-C4'	2.27	107.06	102.64
4	B	2600	AGS	PA-O3A-PB	-2.21	125.23	132.83
4	A	1600	AGS	C2'-C3'-C4'	2.15	106.82	102.64
4	F	6600	AGS	PA-O3A-PB	-2.12	125.56	132.83
4	C	3600	AGS	O3G-PG-O3B	2.10	111.64	104.64
4	E	5600	AGS	PA-O3A-PB	-2.09	125.65	132.83
4	A	1600	AGS	PA-O3A-PB	-2.07	125.72	132.83
4	C	3600	AGS	PA-O3A-PB	-2.05	125.78	132.83
4	B	2600	AGS	O3G-PG-O3B	2.05	111.50	104.64
4	D	4600	AGS	PA-O3A-PB	-2.03	125.87	132.83
5	F	6701	FB	O9-C9-N10	-2.02	119.94	123.32
4	E	5600	AGS	C2'-C3'-C4'	2.01	106.55	102.64

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3600	AGS	C5'-O5'-PA-O3A
4	C	3600	AGS	O4'-C4'-C5'-O5'
4	D	4600	AGS	C5'-O5'-PA-O3A
4	E	5600	AGS	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	F	6600	AGS	C5'-O5'-PA-O3A
5	B	2701	FB	O12-C12-C5A-C5
5	B	2701	FB	C1-C1A-C2A-C2B
5	B	2701	FB	C1-C1A-C2A-O2A
5	B	2701	FB	C1-C1A-C2A-C3A
5	B	2701	FB	O1A-C1A-C2A-C2B
5	B	2701	FB	O1A-C1A-C2A-O2A
5	B	2701	FB	O1A-C1A-C2A-C3A
5	C	3701	FB	O12-C12-C5A-C5
5	C	3701	FB	C1-C1A-C2A-C2B
5	C	3701	FB	C1-C1A-C2A-O2A
5	C	3701	FB	C1-C1A-C2A-C3A
5	C	3701	FB	O1A-C1A-C2A-C2B
5	C	3701	FB	O1A-C1A-C2A-O2A
5	C	3701	FB	O1A-C1A-C2A-C3A
5	D	4701	FB	O12-C12-C5A-C5
5	D	4701	FB	C1-C1A-C2A-C2B
5	D	4701	FB	C1-C1A-C2A-O2A
5	D	4701	FB	C1-C1A-C2A-C3A
5	D	4701	FB	O1A-C1A-C2A-C2B
5	D	4701	FB	O1A-C1A-C2A-O2A
5	D	4701	FB	O1A-C1A-C2A-C3A
5	E	5701	FB	O12-C12-C5A-C5
5	E	5701	FB	C1-C1A-C2A-C2B
5	E	5701	FB	C1-C1A-C2A-O2A
5	E	5701	FB	C1-C1A-C2A-C3A
5	E	5701	FB	O1A-C1A-C2A-C2B
5	E	5701	FB	O1A-C1A-C2A-O2A
5	E	5701	FB	O1A-C1A-C2A-C3A
5	E	5701	FB	C2B-C2A-C3A-O3A
5	E	5701	FB	O2A-C2A-C3A-O3A
5	F	6701	FB	O12-C12-C5A-C5
5	F	6701	FB	C1-C1A-C2A-C2B
5	F	6701	FB	C1-C1A-C2A-O2A
5	F	6701	FB	C1-C1A-C2A-C3A
5	F	6701	FB	O1A-C1A-C2A-C2B
5	F	6701	FB	O1A-C1A-C2A-O2A
5	F	6701	FB	O1A-C1A-C2A-C3A
4	A	1600	AGS	O4'-C4'-C5'-O5'
4	B	2600	AGS	O4'-C4'-C5'-O5'
4	D	4600	AGS	O4'-C4'-C5'-O5'
4	E	5600	AGS	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	F	6600	AGS	O4'-C4'-C5'-O5'
4	B	2600	AGS	C3'-C4'-C5'-O5'
4	A	1600	AGS	C3'-C4'-C5'-O5'
4	D	4600	AGS	C3'-C4'-C5'-O5'
4	E	5600	AGS	C3'-C4'-C5'-O5'
4	F	6600	AGS	C3'-C4'-C5'-O5'
4	A	1600	AGS	C5'-O5'-PA-O3A
4	B	2600	AGS	C5'-O5'-PA-O3A
4	C	3600	AGS	C5'-O5'-PA-O2A
4	D	4600	AGS	C5'-O5'-PA-O2A
4	E	5600	AGS	C5'-O5'-PA-O2A
4	F	6600	AGS	C5'-O5'-PA-O2A
4	A	1600	AGS	PA-O3A-PB-O1B
4	C	3600	AGS	C3'-C4'-C5'-O5'
4	C	3600	AGS	PA-O3A-PB-O1B
4	D	4600	AGS	C5'-O5'-PA-O1A
4	F	6600	AGS	C5'-O5'-PA-O1A
5	E	5701	FB	C1A-C2A-C3A-O3A

There are no ring outliers.

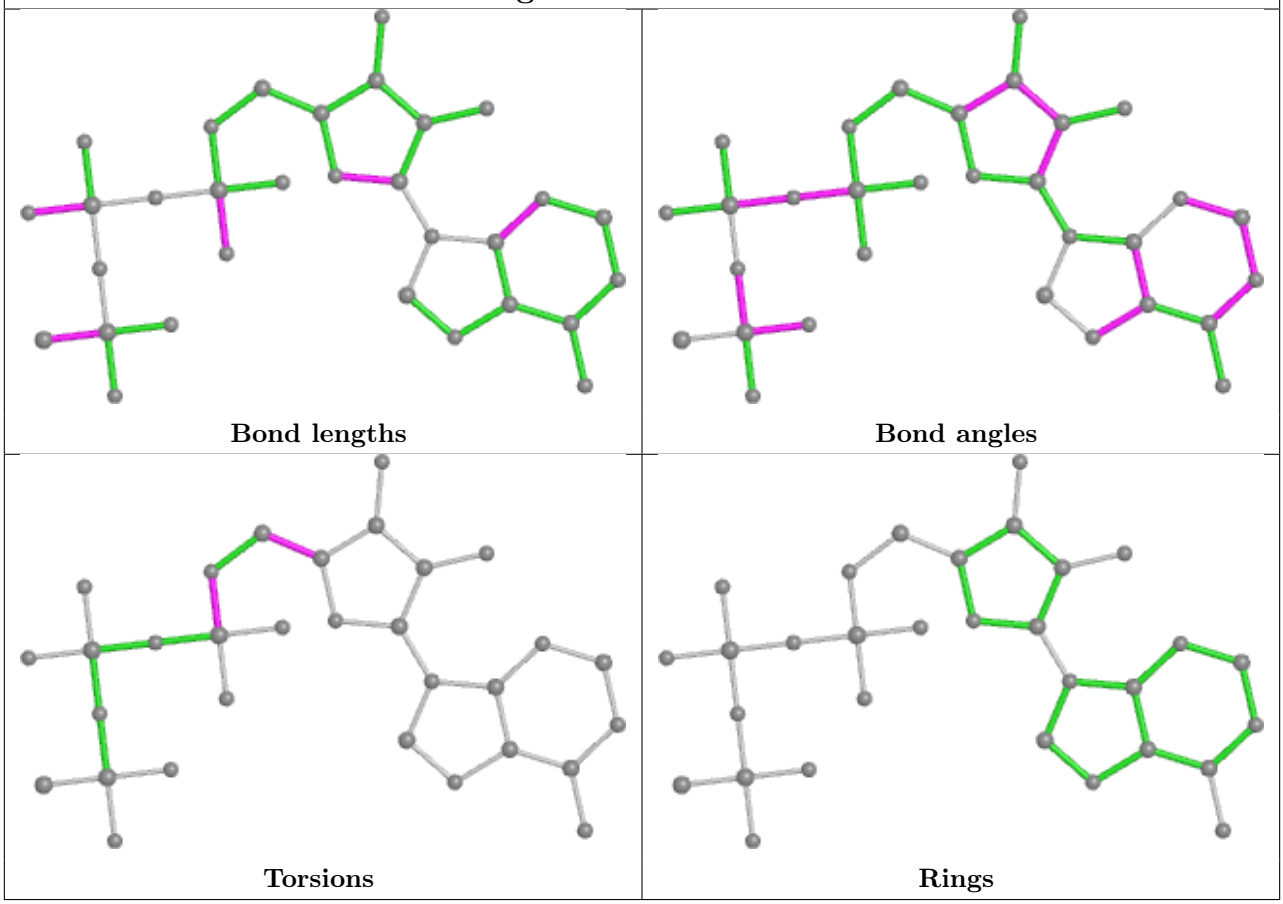
11 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2600	AGS	9	0
5	D	4701	FB	5	0
5	E	5701	FB	8	0
5	F	6701	FB	6	0
4	E	5600	AGS	4	0
4	F	6600	AGS	7	0
4	C	3600	AGS	6	0
4	D	4600	AGS	9	0
5	C	3701	FB	8	0
4	A	1600	AGS	6	0
5	B	2701	FB	4	0

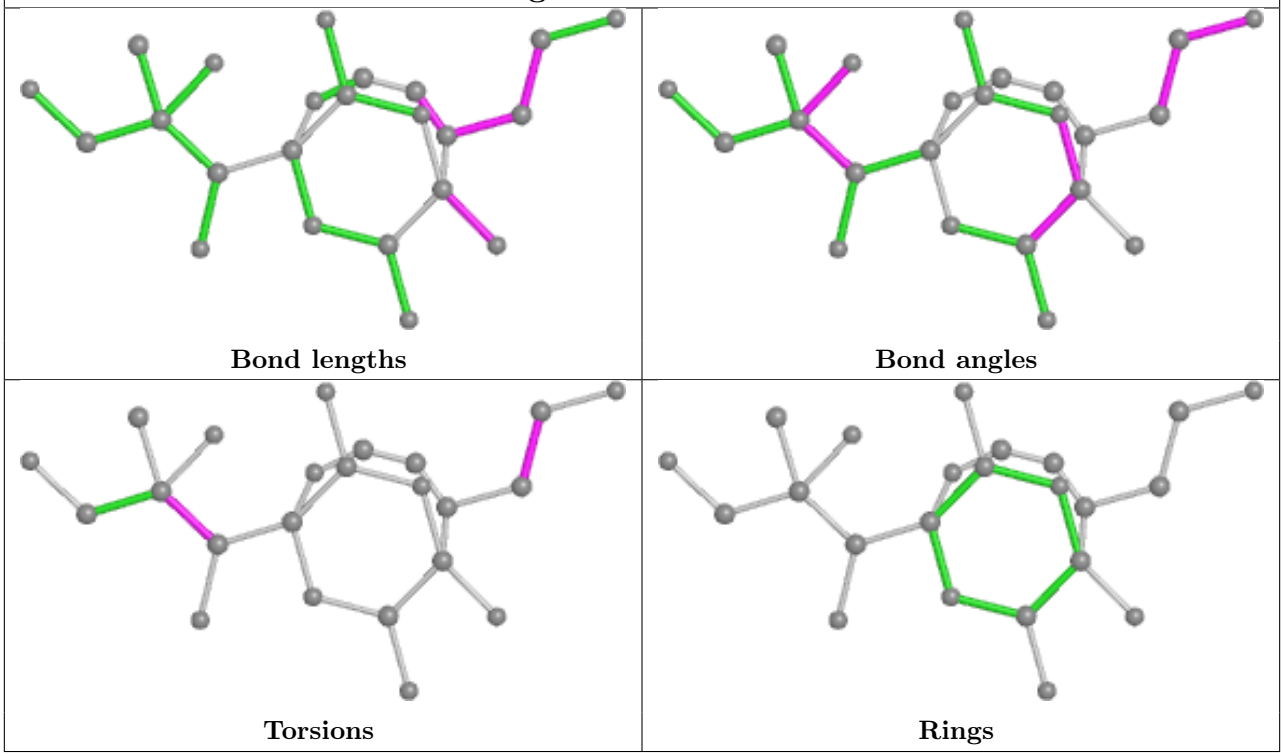
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 AGS B 2600



Ligand FB D 4701



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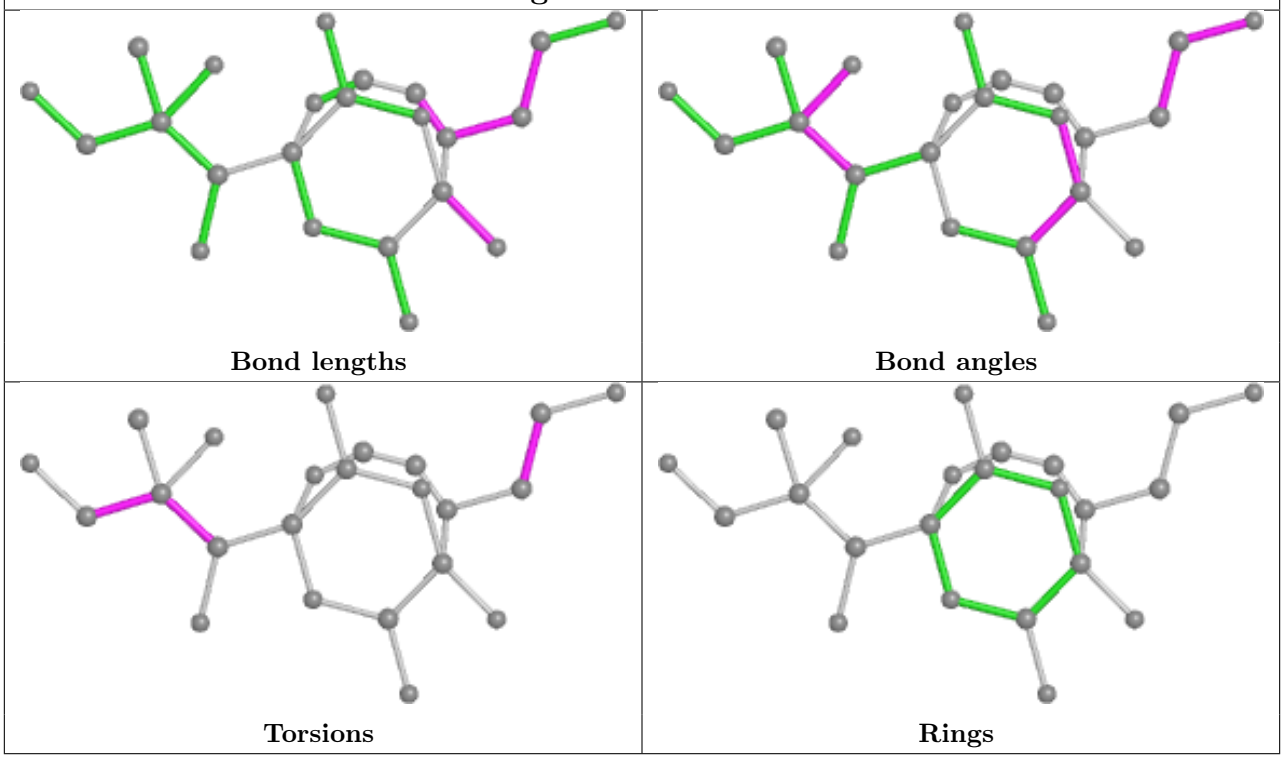

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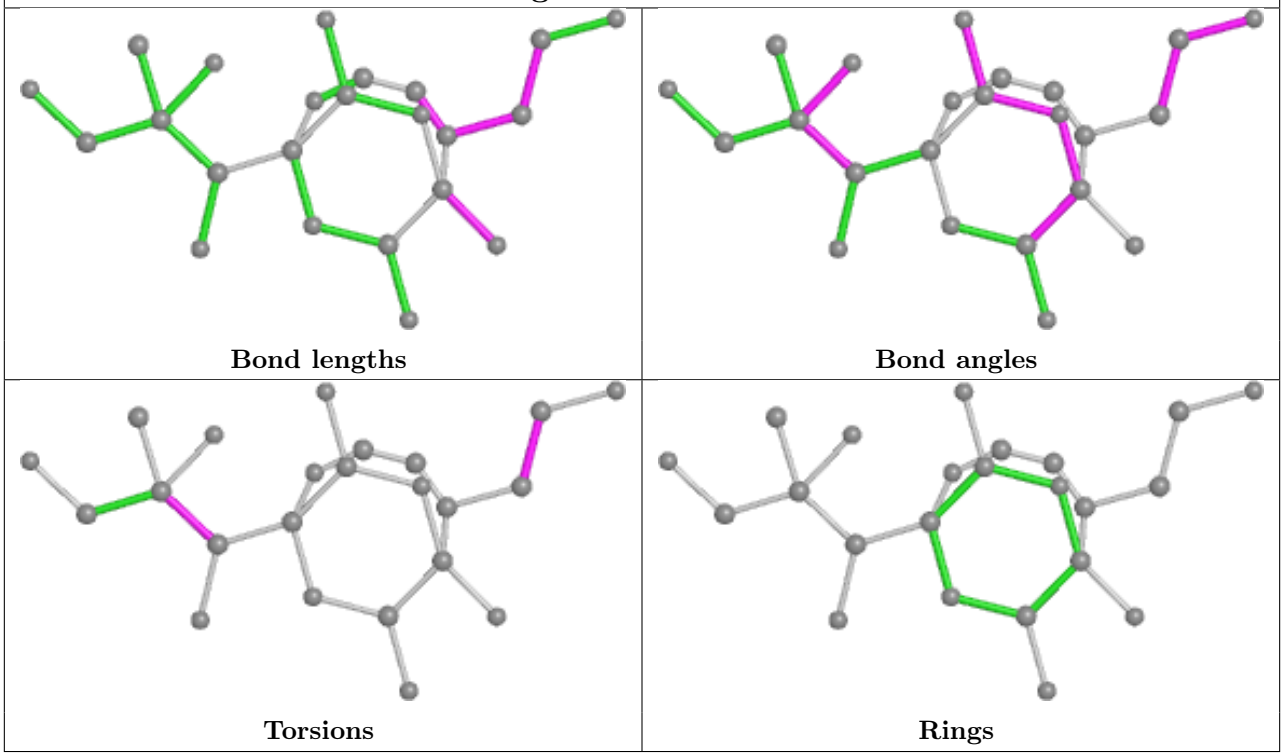

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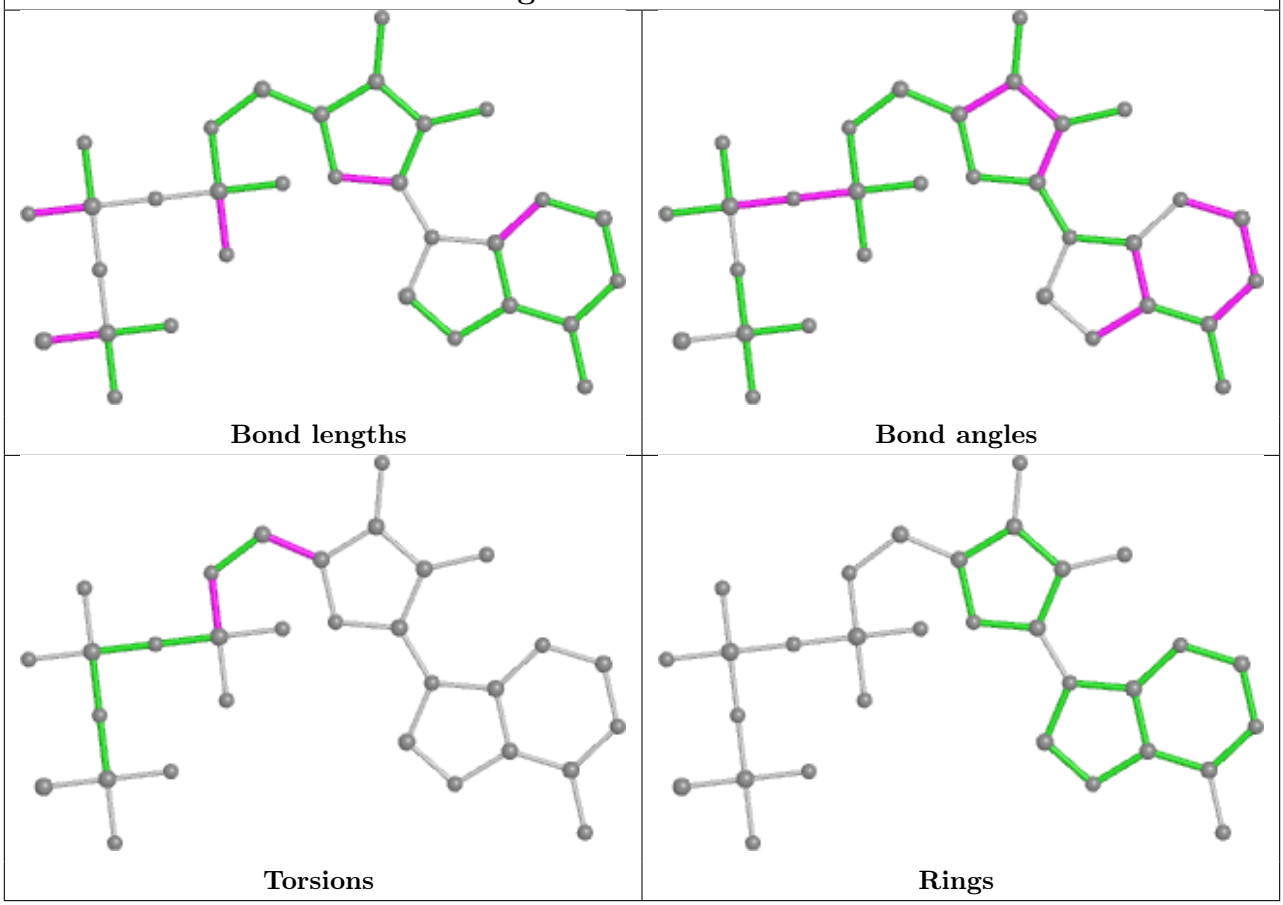

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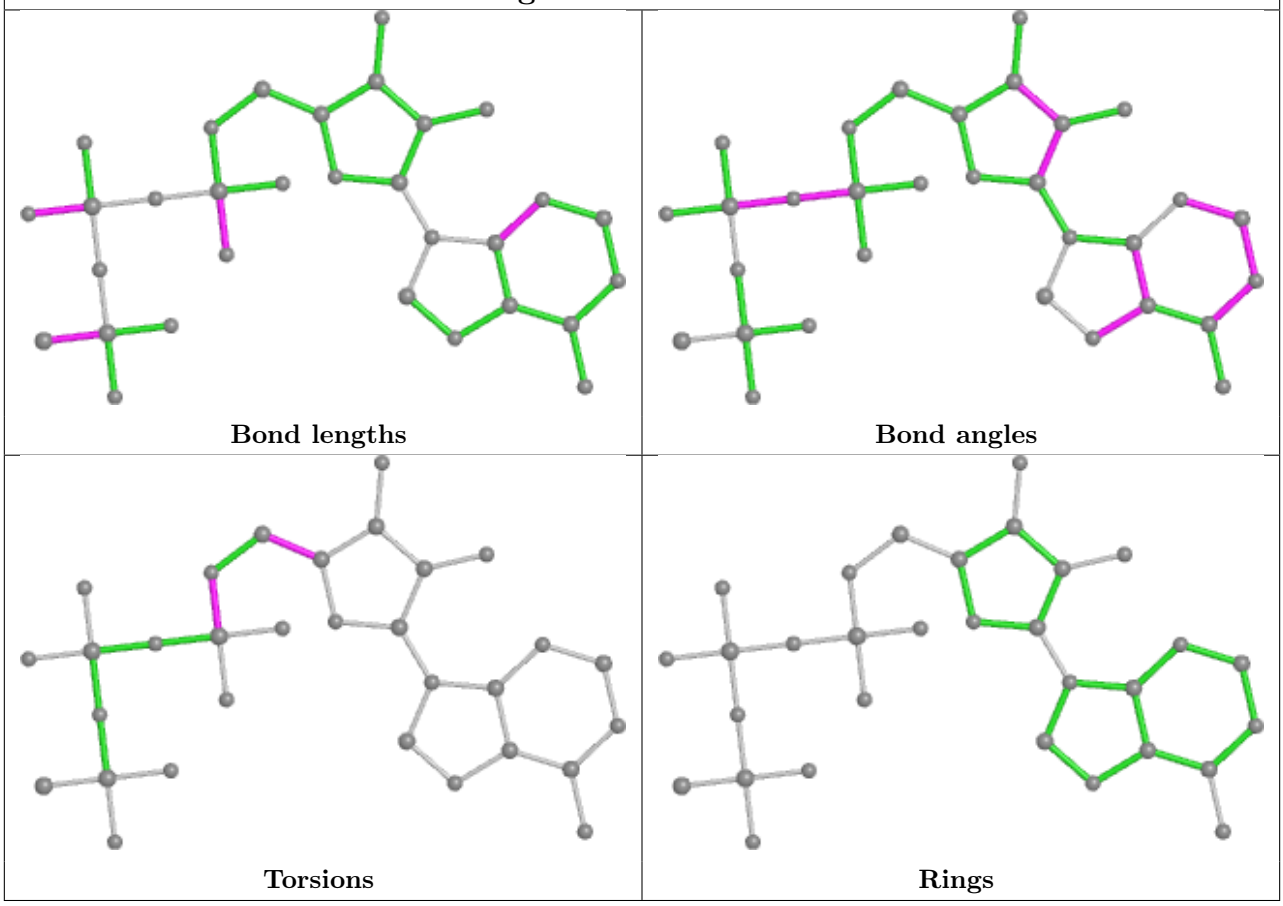
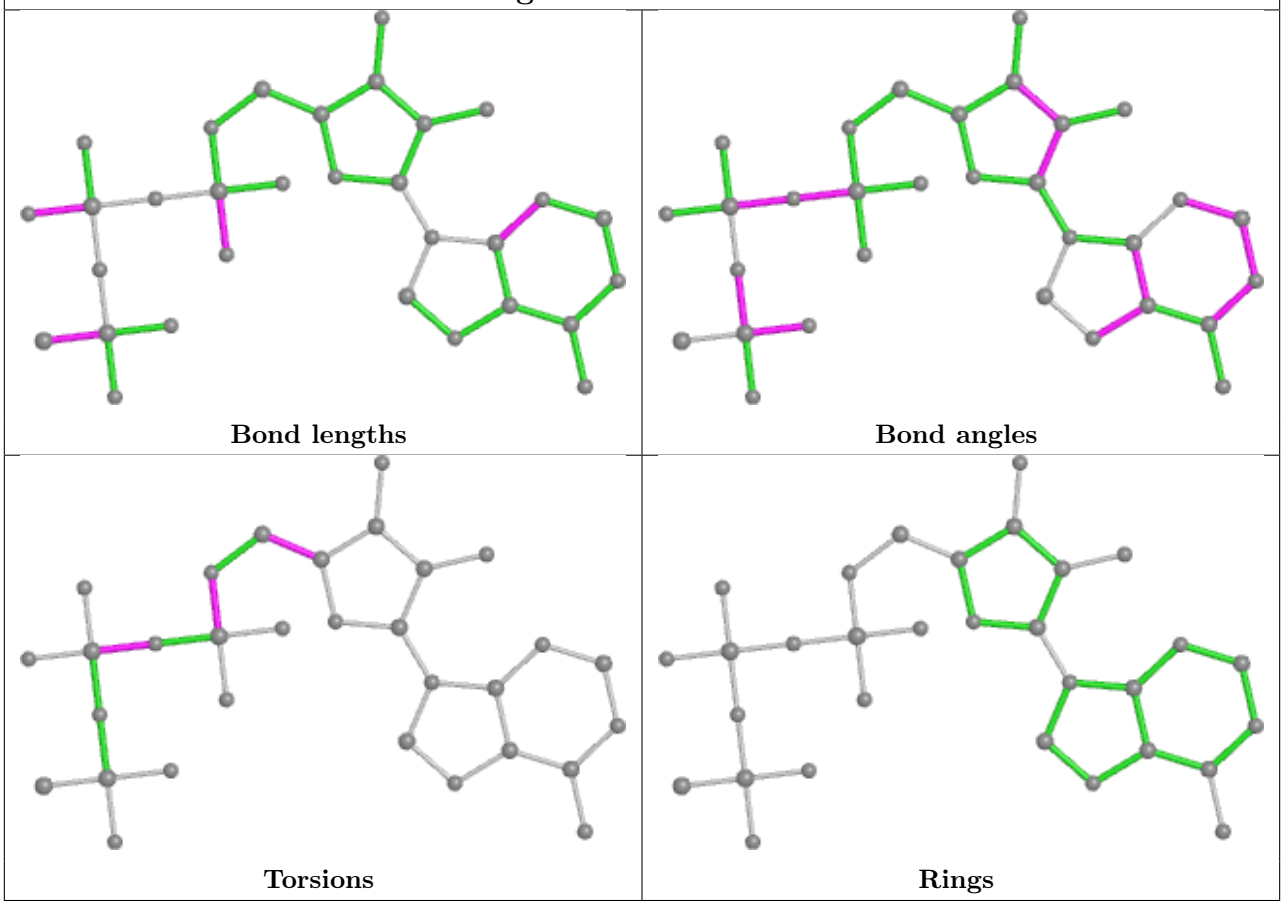
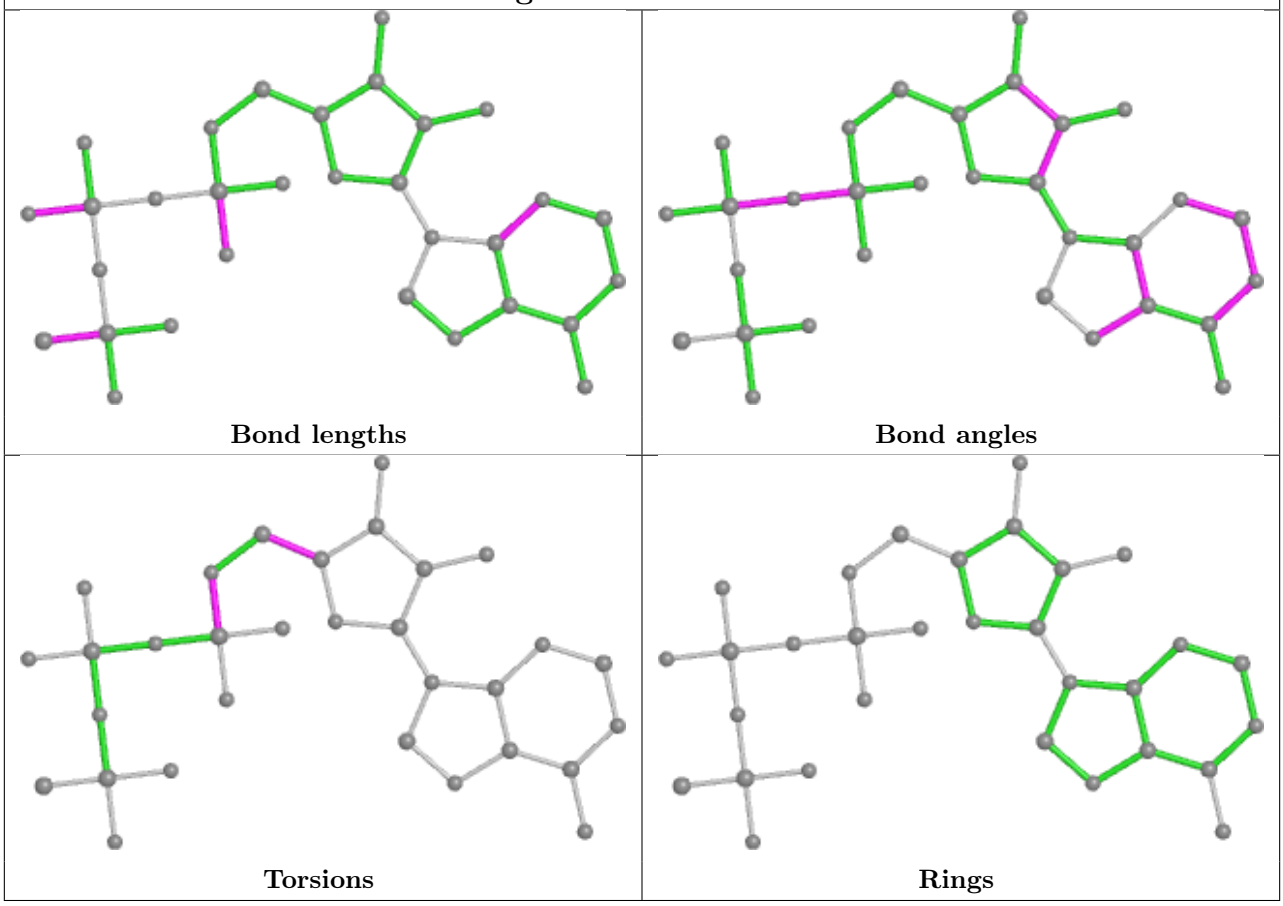


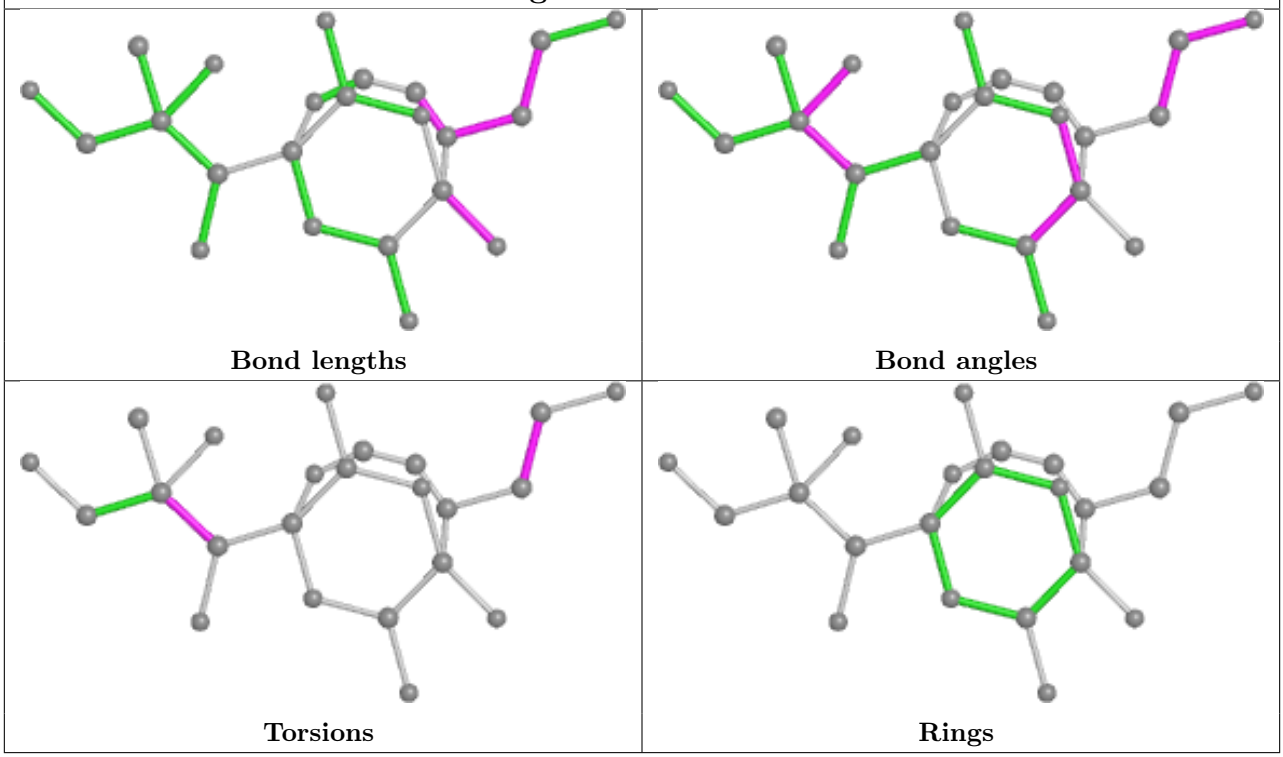
Ligand AGS C 3600



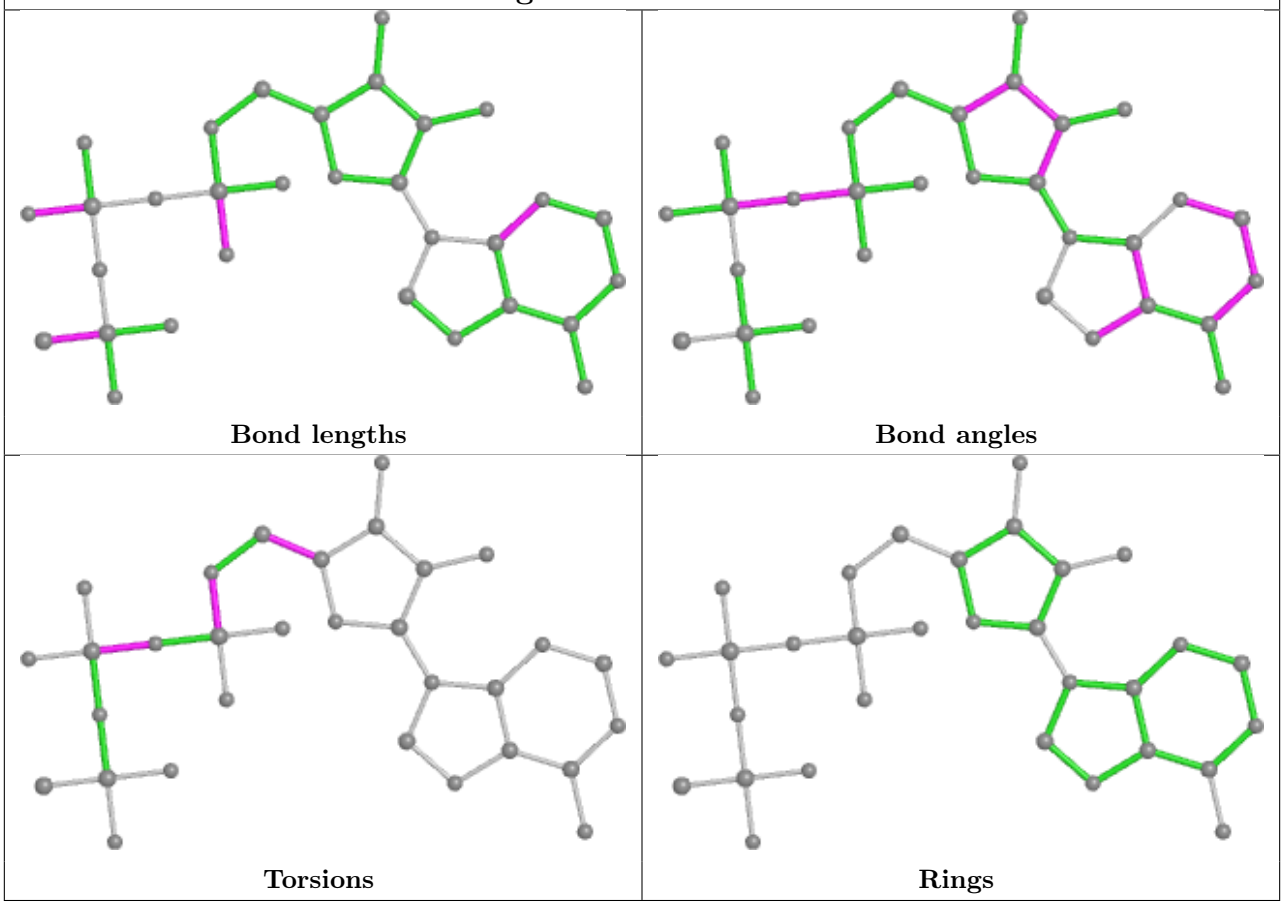
Ligand AGS D 4600



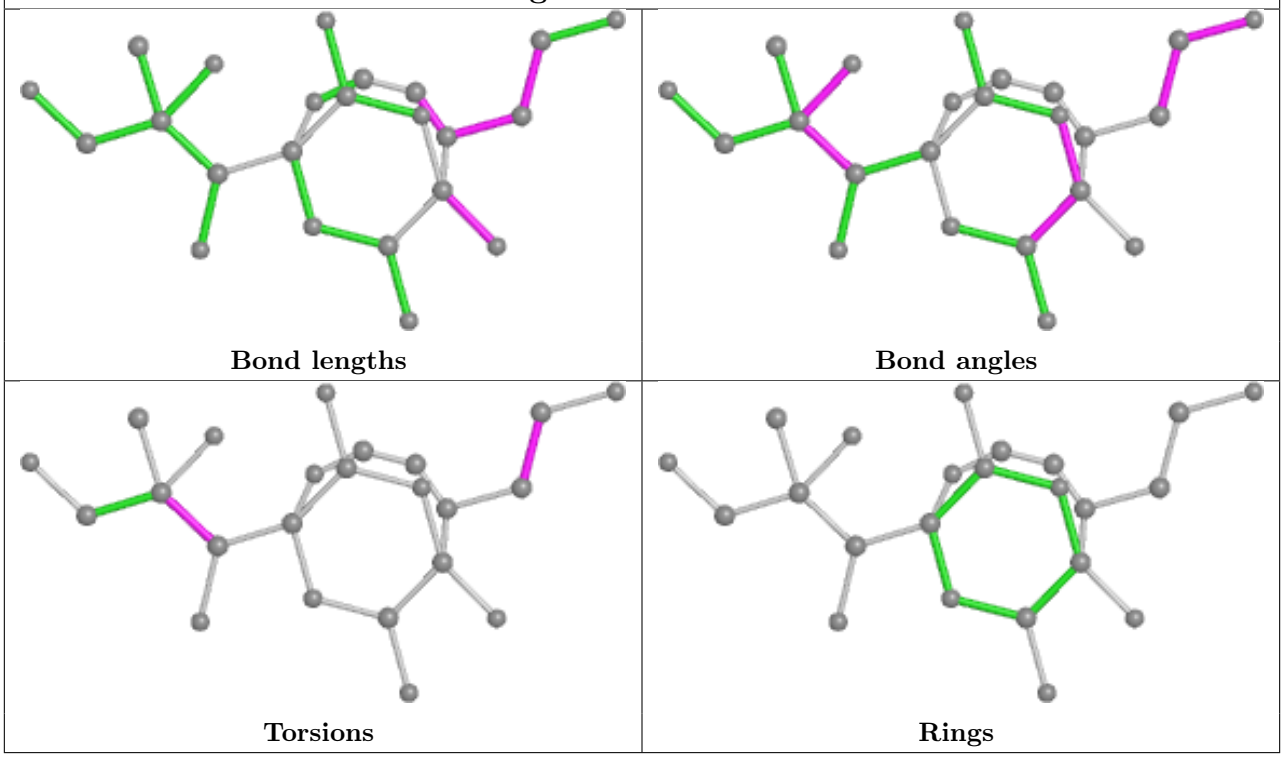
Ligand FB C 3701



Ligand AGS A 1600



Ligand FB B 2701



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%)	6.96	2 (100%)	0	0	123, 123, 123, 123	0
1	H	2/8 (25%)	7.43	2 (100%)	0	0	123, 123, 123, 123	0
1	J	2/8 (25%)	3.34	1 (50%)	0	0	123, 123, 123, 123	0
1	K	2/8 (25%)	3.36	2 (100%)	0	0	123, 123, 123, 123	0
1	L	2/8 (25%)	1.60	0	100	100	122, 122, 122, 122	0
1	M	2/8 (25%)	6.74	2 (100%)	0	0	123, 123, 123, 123	0
2	A	408/419 (97%)	0.15	18 (4%)	34	20	40, 64, 112, 112	0
2	B	408/419 (97%)	-0.00	7 (1%)	70	57	28, 52, 86, 112	0
2	C	408/419 (97%)	-0.17	2 (0%)	91	86	18, 37, 80, 94	0
2	D	408/419 (97%)	-0.01	8 (1%)	65	50	29, 50, 82, 111	0
2	E	407/419 (97%)	0.02	6 (1%)	73	61	28, 50, 90, 112	0
2	F	408/419 (97%)	0.01	13 (3%)	47	30	33, 61, 97, 110	0
All	All	2459/2562 (95%)	0.02	63 (2%)	56	40	18, 54, 105, 123	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	C	8.6
1	M	2	C	8.5
1	G	2	C	8.3
1	H	1	U	6.3
1	G	1	U	5.6
2	A	6	LEU	5.1
1	M	1	U	5.0
1	J	2	C	4.8
1	K	2	C	4.0
2	A	157	LEU	3.9
2	F	140	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	140	HIS	3.7
2	A	280	ALA	3.7
2	F	280	ALA	3.7
2	E	414	GLU	3.5
2	A	286	THR	3.3
2	B	142	ASN	3.2
2	A	374	GLN	3.2
2	D	412	PHE	3.2
2	A	19	GLU	3.1
2	F	98	SER	3.1
2	A	12	SER	3.0
2	A	155	GLU	3.0
2	A	138	PRO	2.9
2	E	24	GLU	2.9
2	C	138	PRO	2.9
2	A	279	PRO	2.9
2	F	287	GLY	2.8
2	F	288	GLY	2.8
2	B	352	LYS	2.7
1	K	1	U	2.7
2	E	417	LYS	2.7
2	B	412	PHE	2.6
2	A	405	MET	2.6
2	D	164	LEU	2.6
2	F	1	MET	2.6
2	A	412	PHE	2.5
2	D	1	MET	2.5
2	A	284	VAL	2.4
2	D	51	GLY	2.4
2	D	91	LEU	2.4
2	A	1	MET	2.4
2	C	1	MET	2.4
2	B	48	ASP	2.4
2	A	126	ASN	2.4
2	B	414	GLU	2.3
2	D	355	PHE	2.3
2	E	91	LEU	2.3
2	A	288	GLY	2.3
2	B	114	LEU	2.3
2	F	284	VAL	2.3
2	F	289	VAL	2.3
2	A	5	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	286	THR	2.2
2	D	60	ASP	2.2
2	B	107	GLY	2.2
2	F	45	SER	2.2
2	F	99	GLY	2.2
2	F	38	ILE	2.1
2	F	285	LEU	2.1
2	D	142	ASN	2.1
2	E	90	ASN	2.0
2	A	389	PRO	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
4	AGS	A	1600	31/31	0.66	0.34	77,80,89,89	0
5	FB	B	2701	23/23	0.66	0.59	43,53,53,53	0
5	FB	F	6701	23/23	0.73	0.45	43,53,53,53	0
5	FB	E	5701	23/23	0.74	0.49	11,43,53,53	0
4	AGS	D	4600	31/31	0.74	0.45	77,79,87,87	0
5	FB	D	4701	23/23	0.75	0.45	11,43,43,53	0
4	AGS	C	3600	31/31	0.77	0.43	77,79,88,88	0
4	AGS	F	6600	31/31	0.77	0.44	76,79,88,88	0
4	AGS	E	5600	31/31	0.79	0.41	77,79,87,87	0
5	FB	C	3701	23/23	0.80	0.39	11,43,43,53	0
3	MG	D	4601	1/1	0.85	0.47	36,36,36,36	0
3	MG	C	3601	1/1	0.86	0.76	77,77,77,77	0
4	AGS	B	2600	31/31	0.89	0.36	77,79,88,88	0

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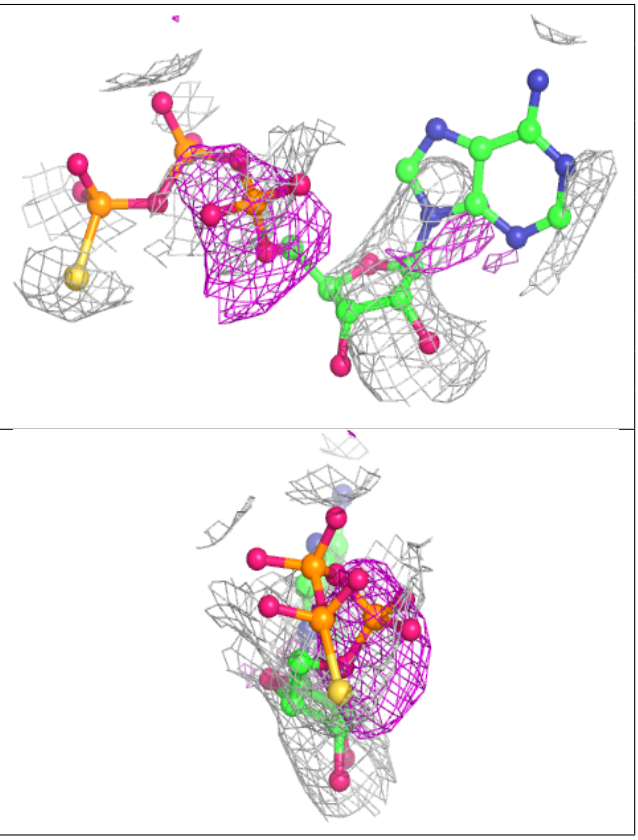
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	F	6601	1/1	0.90	0.58	62,62,62,62	0
3	MG	A	1601	1/1	0.90	0.23	62,62,62,62	0
3	MG	B	2601	1/1	0.95	0.47	59,59,59,59	0
3	MG	E	5601	1/1	0.95	0.63	60,60,60,60	0

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.

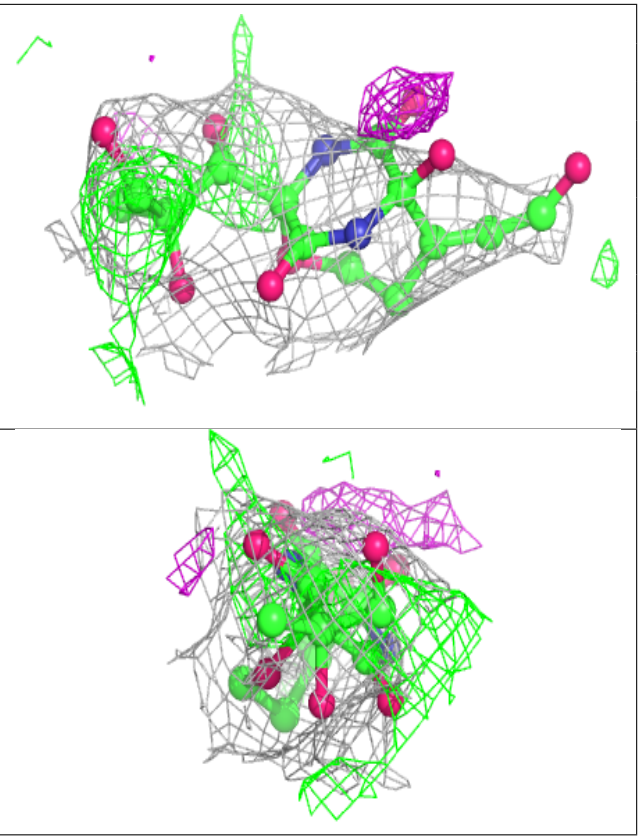
Electron density around AGS A 1600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



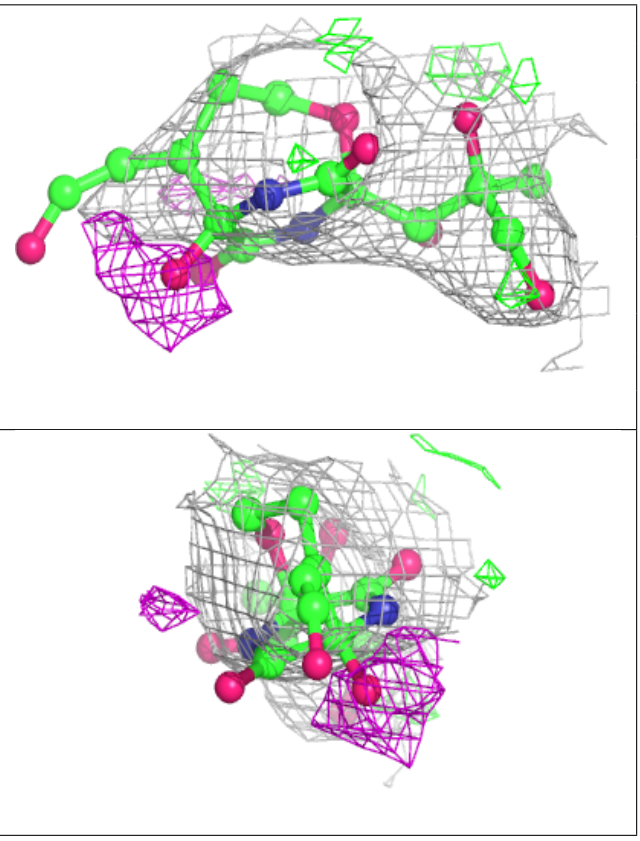
Electron density around FB B 2701:

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



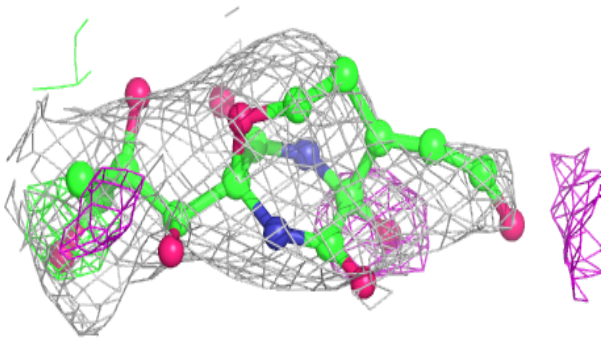
Electron density around FB F 6701:

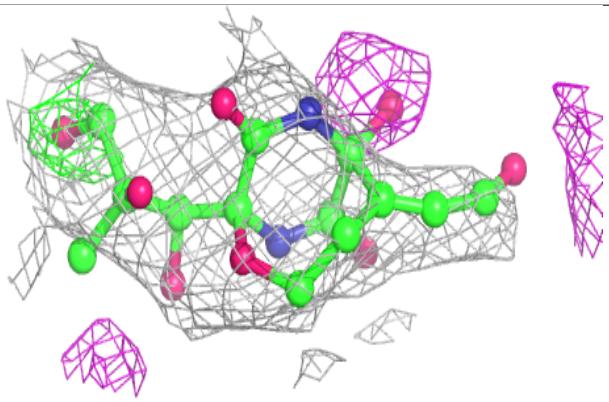
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

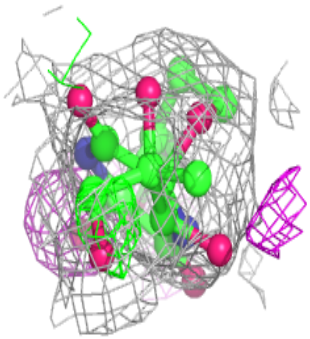


Electron density around FB E 5701:

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

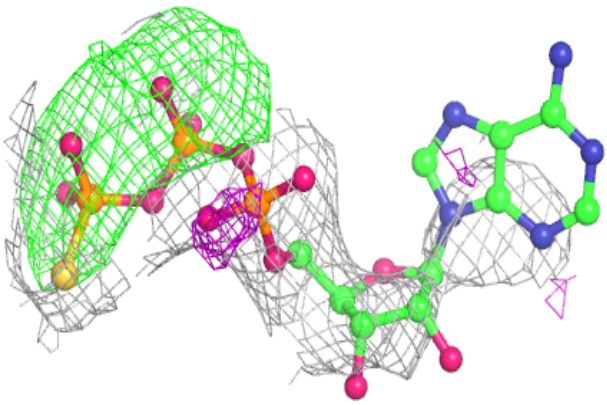


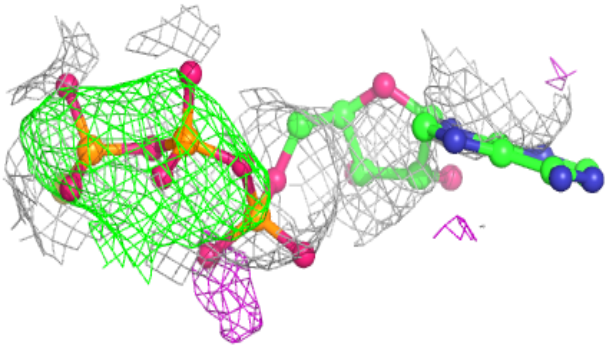


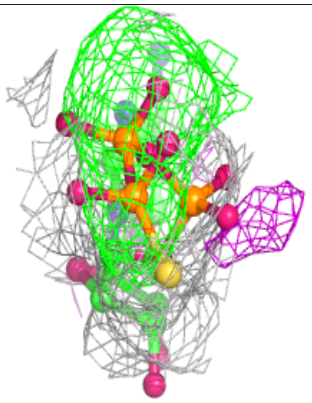


Electron density around AGS D 4600:

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

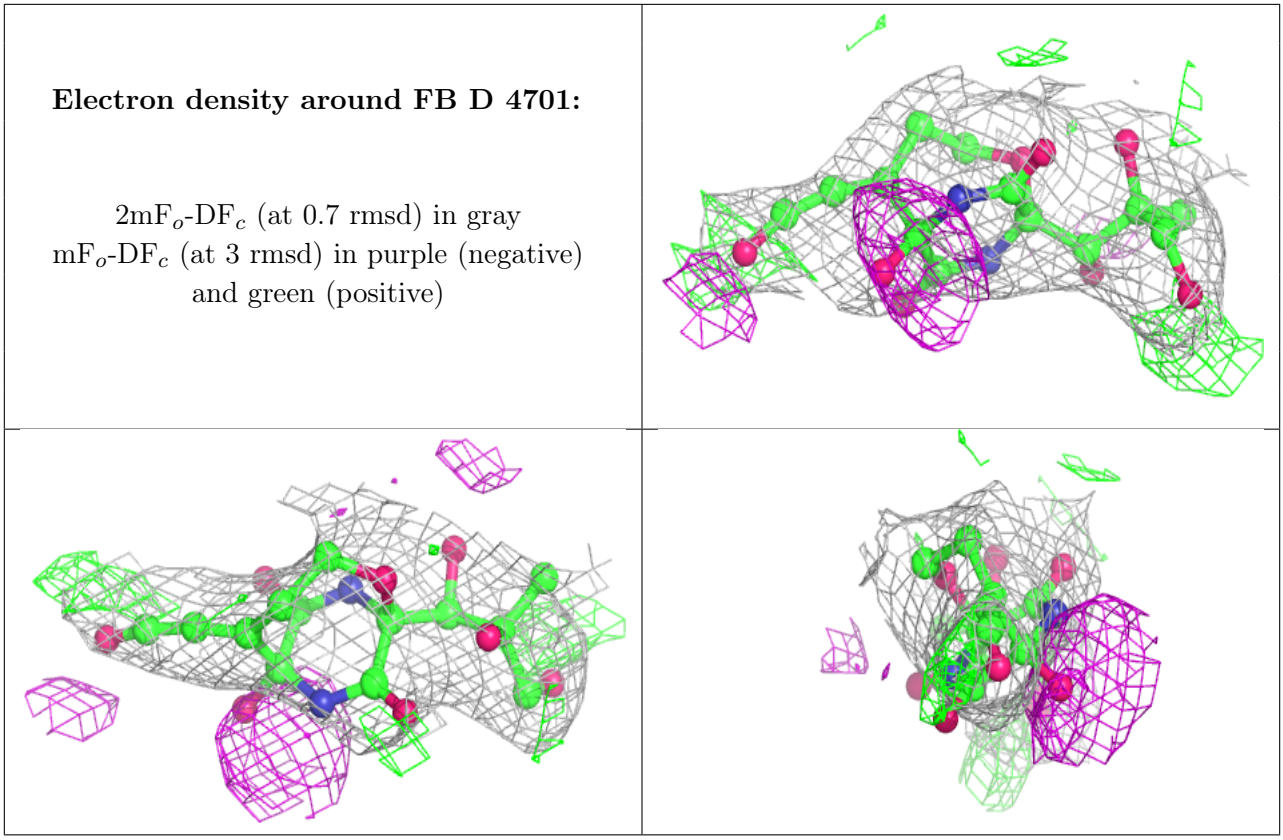






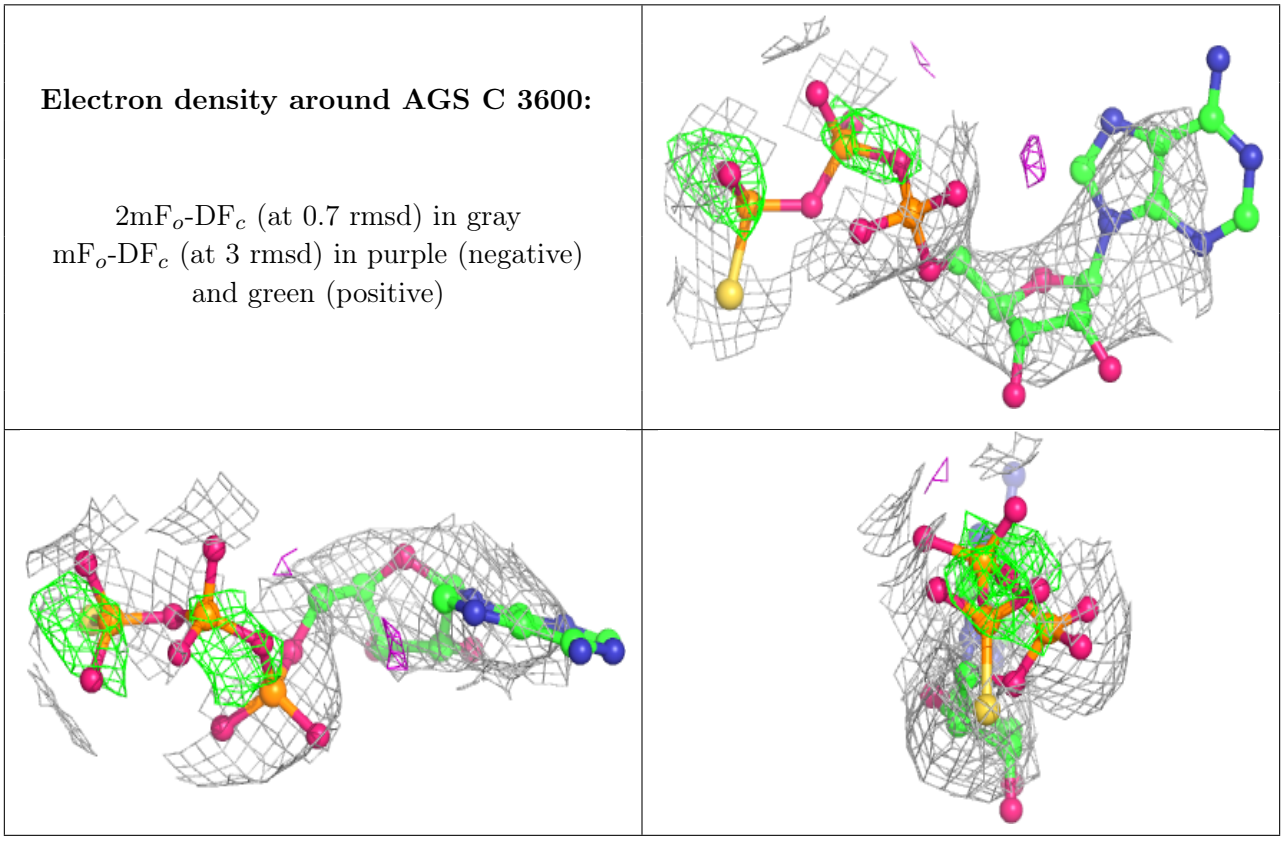
Electron density around FB D 4701:

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



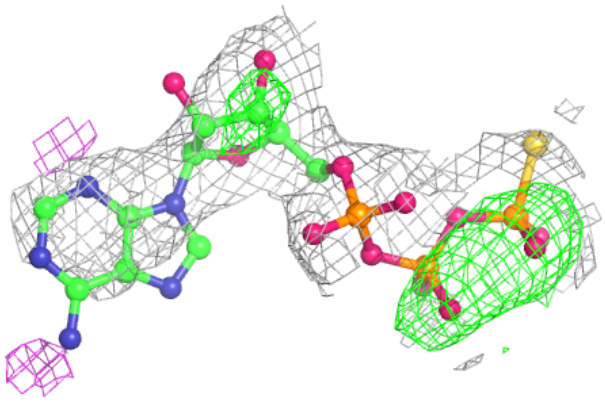
Electron density around AGS C 3600:

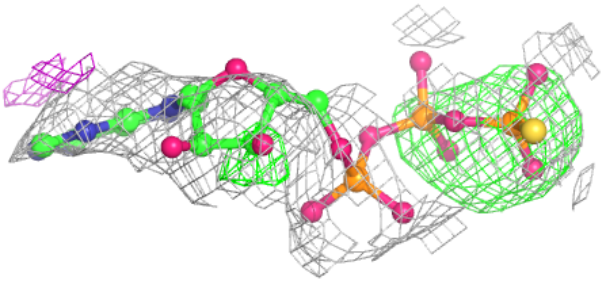
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

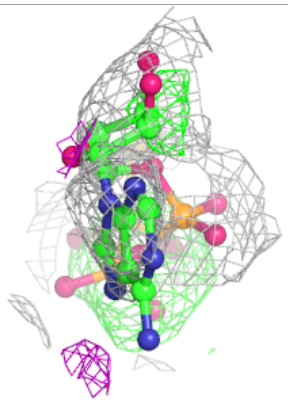


Electron density around AGS F 6600:

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

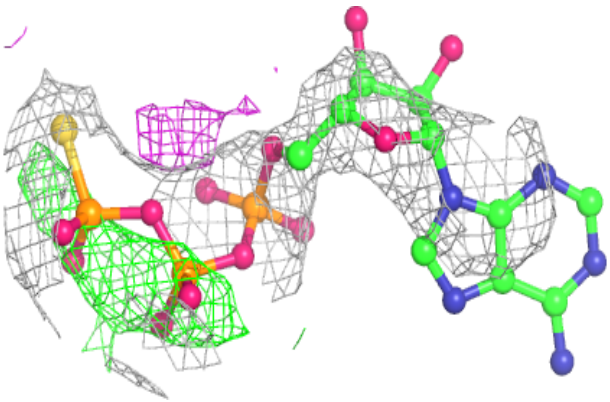


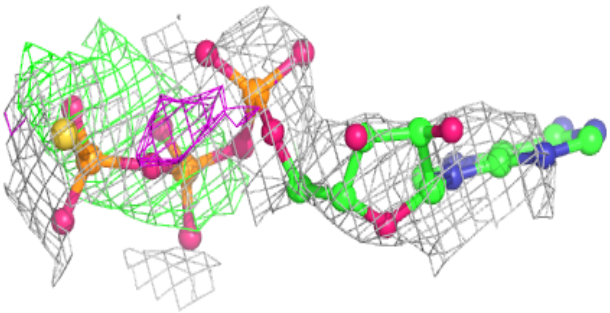


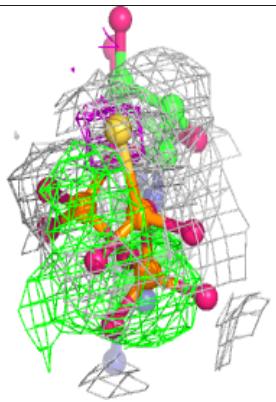


Electron density around AGS E 5600:

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

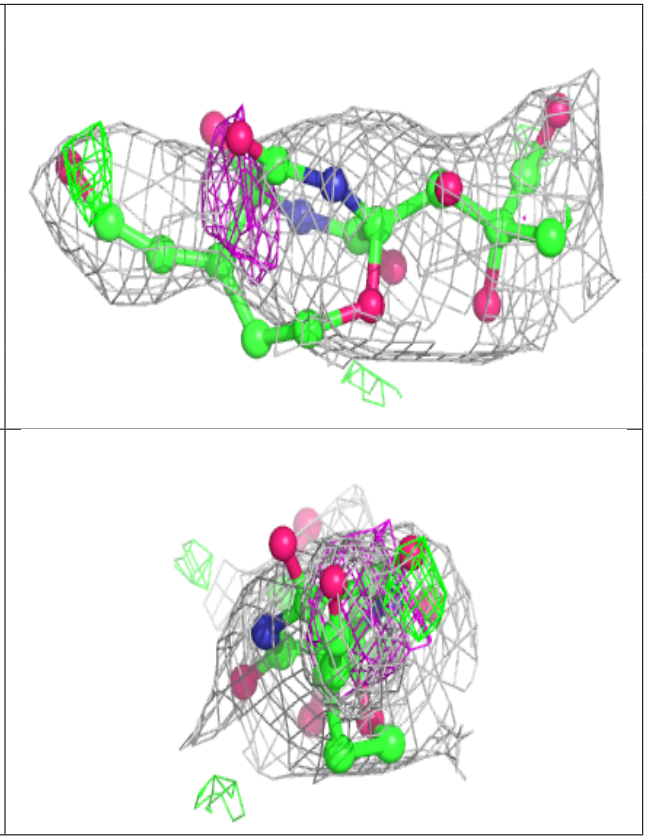






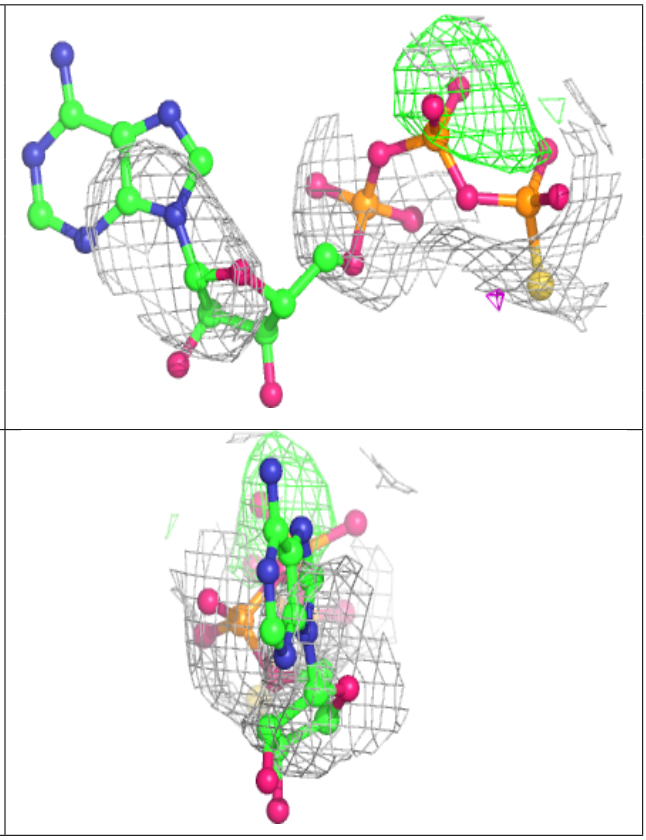
Electron density around FB C 3701:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.