Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2020 – 02:04 pm GMT

PDB ID	:	6TIX
Title	:	Crystal structure of penicillin-binding protein 2 from Yersinia pestis in complex with mecillinam
Authors	:	Pankov, G.; Hunter, W.N.; Dawson, A.
Deposited on	:	2019-11-22
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

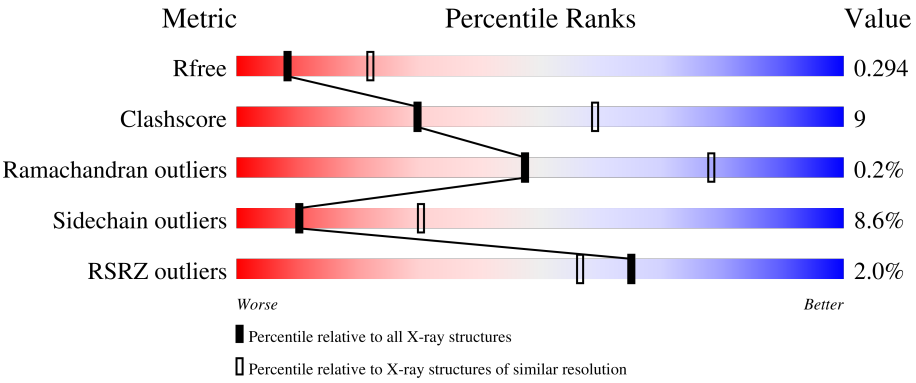
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	AAA	583	3% 63% 20% · 15%
1	BBB	583	% 66% 22% · 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8270 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidoglycan D,D-transpeptidase MrdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	498	Total	C	N	O	S	0	0	0
			3908	2496	671	733	8			
1	BBB	533	Total	C	N	O	S	0	0	0
			4214	2684	740	781	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	31	HIS	-	expression tag	UNP A0A384KFW3
AAA	32	HIS	-	expression tag	UNP A0A384KFW3
AAA	33	HIS	-	expression tag	UNP A0A384KFW3
AAA	34	HIS	-	expression tag	UNP A0A384KFW3
AAA	35	HIS	-	expression tag	UNP A0A384KFW3
AAA	36	HIS	-	expression tag	UNP A0A384KFW3
AAA	37	SER	-	expression tag	UNP A0A384KFW3
AAA	38	SER	-	expression tag	UNP A0A384KFW3
AAA	39	GLY	-	expression tag	UNP A0A384KFW3
AAA	40	GLU	-	expression tag	UNP A0A384KFW3
AAA	41	ASN	-	expression tag	UNP A0A384KFW3
AAA	42	LEU	-	expression tag	UNP A0A384KFW3
AAA	43	TYR	-	expression tag	UNP A0A384KFW3
AAA	44	PHE	-	expression tag	UNP A0A384KFW3
AAA	45	GLN	-	expression tag	UNP A0A384KFW3
AAA	46	GLY	-	expression tag	UNP A0A384KFW3
AAA	47	HIS	-	expression tag	UNP A0A384KFW3
AAA	48	MET	-	expression tag	UNP A0A384KFW3
BBB	31	HIS	-	expression tag	UNP A0A384KFW3
BBB	32	HIS	-	expression tag	UNP A0A384KFW3
BBB	33	HIS	-	expression tag	UNP A0A384KFW3
BBB	34	HIS	-	expression tag	UNP A0A384KFW3
BBB	35	HIS	-	expression tag	UNP A0A384KFW3
BBB	36	HIS	-	expression tag	UNP A0A384KFW3
BBB	37	SER	-	expression tag	UNP A0A384KFW3

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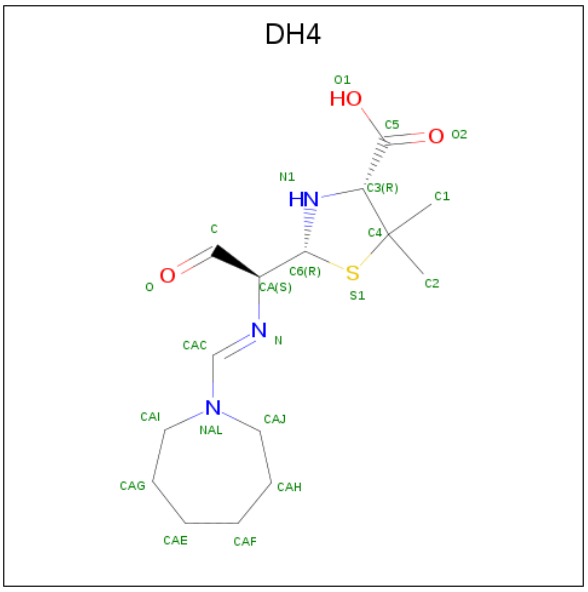
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	38	SER	-	expression tag	UNP A0A384KFW3
BBB	39	GLY	-	expression tag	UNP A0A384KFW3
BBB	40	GLU	-	expression tag	UNP A0A384KFW3
BBB	41	ASN	-	expression tag	UNP A0A384KFW3
BBB	42	LEU	-	expression tag	UNP A0A384KFW3
BBB	43	TYR	-	expression tag	UNP A0A384KFW3
BBB	44	PHE	-	expression tag	UNP A0A384KFW3
BBB	45	GLN	-	expression tag	UNP A0A384KFW3
BBB	46	GLY	-	expression tag	UNP A0A384KFW3
BBB	47	HIS	-	expression tag	UNP A0A384KFW3
BBB	48	MET	-	expression tag	UNP A0A384KFW3

- Molecule 2 is 2-[(1R)-1-{[(E)-azepan-1-ylmethylidene]amino}-2-oxoethyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxylic acid (three-letter code: DH4) (formula: $C_{15}H_{25}N_3O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
2	BBB	1	Total	C	N	O	S	0	0
			22	15	3	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	50	Total	O	0	0
			50	50		

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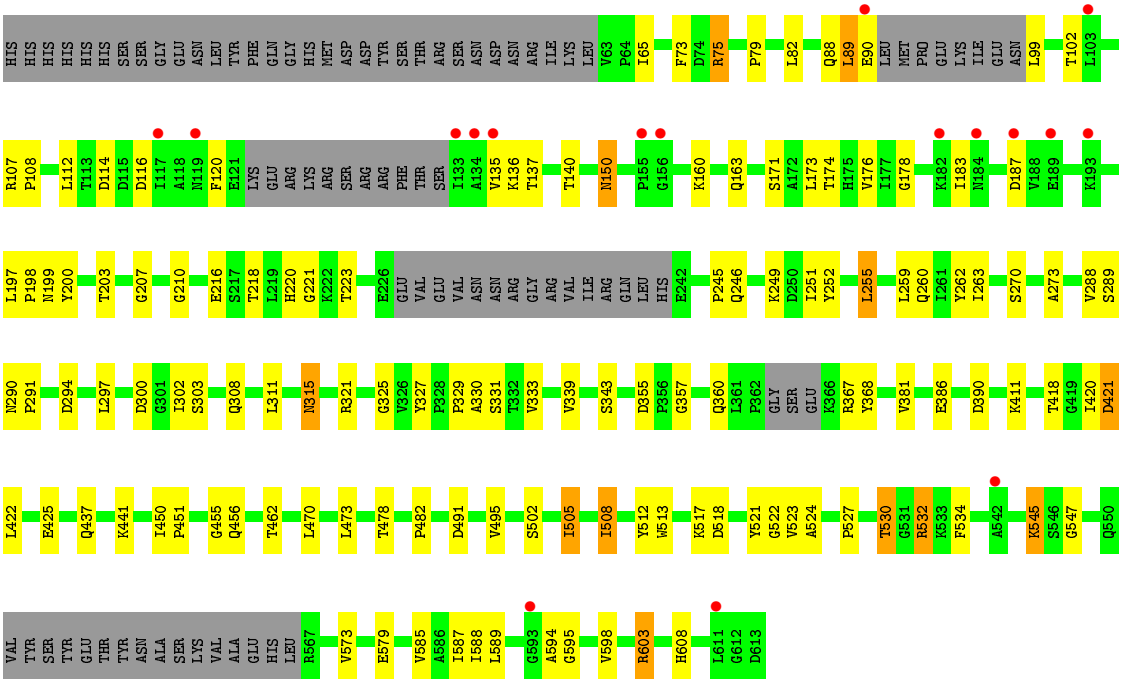
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	54	Total	O	0	0
			54	54		

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.

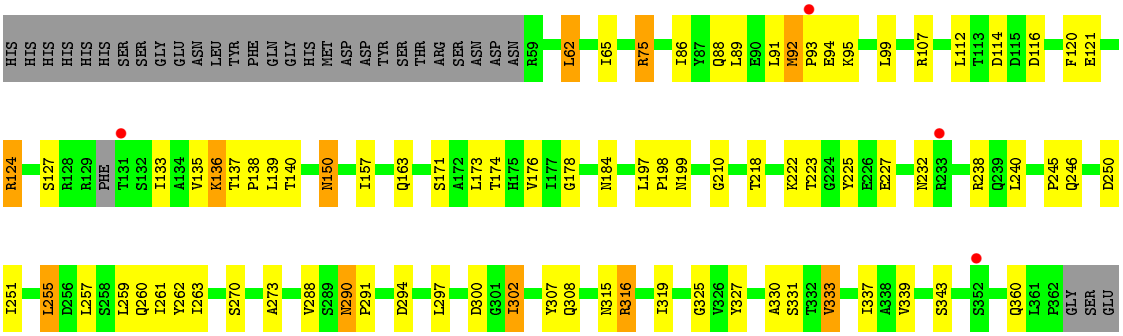
- Molecule 1: Peptidoglycan D,D-transpeptidase MrdA

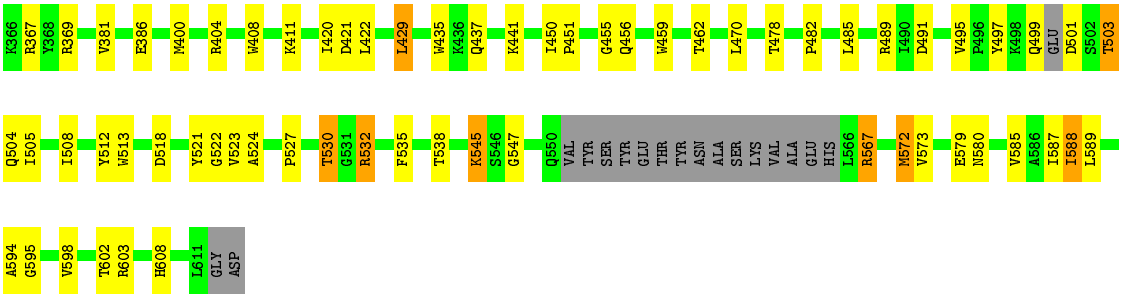
Chain AAA:



- Molecule 1: Peptidoglycan D,D-transpeptidase MrdA

Chain BBB:




K366 R367 Y368 R369 V381 E386 M400 R404 W408 K411 I420 D421 L422 L429 W435 K436 Q437 K441 I450 P451 G455 Q456 W459 T462 L470 T478 P482 L485 R489 I490 D491 V495 P496 Y497 K498 Q499 GLU D501 S502 T503
Q504 I505 I508 Y512 W513 D518 Y521 G522 V523 A524 P527 T530 G531 R532 F535 T538 K545 S546 G547 Q550 VAL TYR SER TYR GLU THR TYR ASN ALA SER LYS VAL ALA GLU HIS L566 R567 M572 V573 E579 N580 V585 A586 I587 I588 L589
A594 G595 V598 T602 R603 H608 L611 GLY ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.17Å 84.03Å 87.10Å 112.92° 95.31° 104.57°	Depositor
Resolution (Å)	45.69 – 2.80 45.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.4 (45.69-2.80) 92.5 (45.65-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.290 0.238 , 0.294	Depositor DCC
R_{free} test set	1308 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8270	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DH4

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	AAA	0.63	0/3999	0.76	0/5430
1	BBB	0.64	0/4308	0.77	0/5841
All	All	0.63	0/8307	0.77	0/11271

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3908	0	3881	72	0
1	BBB	4214	0	4228	84	0
2	AAA	22	0	23	2	0
2	BBB	22	0	23	1	0
3	AAA	50	0	0	2	0
3	BBB	54	0	0	0	0
All	All	8270	0	8155	154	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 (154) 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)
1:AAA:473:LEU:O	1:AAA:517:LYS:HE2	1.88	0.72
1:AAA:75:ARG:HG2	1:AAA:255:LEU:O	1.90	0.72
1:BBB:75:ARG:HG2	1:BBB:255:LEU:O	1.93	0.68
1:AAA:390:ASP:OD2	2:AAA:701:DH4:H13	1.94	0.67
1:BBB:411:LYS:HB3	1:BBB:505:ILE:HG21	1.75	0.66
1:BBB:524:ALA:O	1:BBB:532:ARG:HA	2.00	0.62
1:AAA:524:ALA:O	1:AAA:532:ARG:HA	2.00	0.61
1:BBB:527:PRO:O	1:BBB:532:ARG:NE	2.28	0.61
1:BBB:92:MET:HB3	1:BBB:95:LYS:HB2	1.82	0.61
1:AAA:534:PHE:O	1:AAA:603:ARG:HG3	2.01	0.60
1:BBB:470:LEU:HD22	1:BBB:573:VAL:HB	1.82	0.60
1:AAA:289:SER:HB3	3:AAA:803:HOH:O	2.02	0.60
1:AAA:270:SER:HB3	1:AAA:594:ALA:HB2	1.86	0.57
1:BBB:251:ILE:HD12	1:BBB:485:LEU:HD13	1.85	0.57
1:BBB:199:ASN:O	1:BBB:223:THR:OG1	2.23	0.57
1:AAA:470:LEU:HD22	1:AAA:573:VAL:HB	1.86	0.57
1:AAA:176:VAL:HG21	1:AAA:255:LEU:HD11	1.86	0.56
1:BBB:263:ILE:HB	1:BBB:288:VAL:HG21	1.88	0.55
1:AAA:199:ASN:O	1:AAA:223:THR:OG1	2.24	0.55
1:AAA:508:ILE:H	1:AAA:508:ILE:HD13	1.69	0.55
1:AAA:527:PRO:O	1:AAA:532:ARG:NH1	2.40	0.55
1:BBB:89:LEU:HB2	1:BBB:139:LEU:HD11	1.89	0.55
1:BBB:173:LEU:CD2	1:BBB:260:GLN:HG2	2.36	0.54
1:BBB:567:ARG:HD2	1:BBB:567:ARG:H	1.72	0.54
1:AAA:150:ASN:N	1:AAA:150:ASN:HD22	2.05	0.54
1:AAA:90:GLU:CD	1:AAA:160:LYS:HG3	2.28	0.54
1:BBB:587:ILE:HD11	1:BBB:589:LEU:HD21	1.90	0.54
1:AAA:368:TYR:CD2	1:AAA:450:ILE:HG21	2.44	0.53
1:AAA:173:LEU:CD2	1:AAA:260:GLN:HG2	2.38	0.53
1:AAA:331:SER:N	2:AAA:701:DH4:O	2.42	0.53
1:BBB:331:SER:N	2:BBB:701:DH4:O	2.42	0.53
1:BBB:62:LEU:CD2	1:BBB:225:TYR:HB3	2.39	0.53
1:AAA:587:ILE:HD11	1:AAA:589:LEU:HD21	1.91	0.53
1:AAA:491:ASP:O	1:BBB:163:GLN:NE2	2.35	0.52
1:BBB:535:PHE:CE1	1:BBB:572:MET:HE1	2.45	0.52
1:BBB:508:ILE:H	1:BBB:508:ILE:HD12	1.74	0.52
1:BBB:270:SER:HB3	1:BBB:594:ALA:HB2	1.92	0.52
1:AAA:263:ILE:HB	1:AAA:288:VAL:HG21	1.92	0.52
1:AAA:331:SER:HB2	1:AAA:547:GLY:HA2	1.91	0.52
1:BBB:176:VAL:HG21	1:BBB:255:LEU:HD11	1.91	0.52
1:BBB:331:SER:HB2	1:BBB:547:GLY:HA2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:93:PRO:HG3	1:BBB:133:ILE:HD13	1.91	0.51
1:BBB:302:ILE:CG2	1:BBB:307:TYR:HB2	2.40	0.51
1:BBB:88:GLN:HG2	1:BBB:137:THR:HB	1.92	0.51
1:BBB:535:PHE:HE1	1:BBB:572:MET:HE1	1.76	0.51
1:BBB:150:ASN:N	1:BBB:150:ASN:HD22	2.09	0.51
1:BBB:333:VAL:CG2	1:BBB:459:TRP:CH2	2.93	0.51
1:AAA:523:VAL:HG13	1:AAA:530:THR:OG1	2.11	0.51
1:AAA:65:ILE:HG22	1:AAA:245:PRO:HG3	1.93	0.50
1:AAA:518:ASP:O	1:AAA:521:TYR:HB3	2.12	0.50
1:AAA:339:VAL:HG11	1:AAA:513:TRP:CZ3	2.47	0.49
1:BBB:121:GLU:HA	1:BBB:124:ARG:CG	2.41	0.49
1:BBB:518:ASP:O	1:BBB:521:TYR:HB3	2.13	0.49
1:BBB:523:VAL:HG13	1:BBB:530:THR:OG1	2.13	0.49
1:BBB:294:ASP:HB3	1:BBB:297:LEU:HG	1.95	0.49
1:BBB:65:ILE:HG22	1:BBB:245:PRO:HG3	1.94	0.49
1:BBB:429:LEU:HD21	1:BBB:435:TRP:CZ2	2.47	0.48
1:BBB:171:SER:HA	1:BBB:174:THR:OG1	2.14	0.48
1:AAA:450:ILE:HB	1:AAA:451:PRO:HD3	1.95	0.48
1:BBB:227:GLU:HB3	1:BBB:240:LEU:HB2	1.96	0.48
1:BBB:339:VAL:HG11	1:BBB:513:TRP:CZ3	2.48	0.48
1:AAA:259:LEU:O	1:AAA:263:ILE:HG12	2.13	0.48
1:BBB:222:LYS:HB2	1:BBB:246:GLN:HB2	1.96	0.47
1:BBB:259:LEU:O	1:BBB:263:ILE:HG12	2.13	0.47
1:BBB:95:LYS:HE2	1:BBB:232:ASN:O	2.15	0.47
1:AAA:120:PHE:CD1	1:AAA:135:VAL:HA	2.49	0.47
1:BBB:450:ILE:HB	1:BBB:451:PRO:HD3	1.96	0.47
1:AAA:203:THR:HG21	1:AAA:220:HIS:CE1	2.50	0.46
1:AAA:163:GLN:NE2	1:BBB:491:ASP:O	2.47	0.46
1:AAA:171:SER:HA	1:AAA:174:THR:OG1	2.15	0.46
1:BBB:333:VAL:HG11	1:BBB:459:TRP:CZ3	2.50	0.46
1:AAA:116:ASP:OD2	1:AAA:136:LYS:NZ	2.49	0.46
1:AAA:88:GLN:HG2	1:AAA:137:THR:HB	1.97	0.46
1:BBB:107:ARG:HA	1:BBB:112:LEU:HB3	1.96	0.46
1:BBB:250:ASP:HB2	1:BBB:489:ARG:HB3	1.96	0.46
1:BBB:120:PHE:CD1	1:BBB:135:VAL:HA	2.50	0.46
1:AAA:291:PRO:HG3	1:AAA:315:ASN:HB3	1.98	0.46
1:AAA:331:SER:HB3	1:AAA:545:LYS:NZ	2.31	0.46
1:BBB:333:VAL:HG21	1:BBB:459:TRP:CH2	2.50	0.46
1:AAA:343:SER:HA	1:AAA:512:TYR:HE2	1.81	0.46
1:AAA:289:SER:OG	1:AAA:321:ARG:N	2.49	0.45
1:AAA:273:ALA:HA	1:AAA:288:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:173:LEU:HD23	1:AAA:260:GLN:HG2	1.99	0.45
1:AAA:262:TYR:CD2	1:AAA:608:HIS:ND1	2.85	0.45
1:AAA:221:GLY:HA2	3:AAA:843:HOH:O	2.16	0.45
1:BBB:112:LEU:HD12	1:BBB:116:ASP:HB2	1.98	0.45
1:BBB:91:LEU:HB3	1:BBB:157:ILE:HG12	1.99	0.45
1:BBB:331:SER:HB3	1:BBB:545:LYS:NZ	2.31	0.45
1:AAA:107:ARG:HB2	1:AAA:108:PRO:HD3	1.99	0.45
1:AAA:174:THR:O	1:AAA:178:GLY:HA2	2.17	0.45
1:BBB:136:LYS:HD2	1:BBB:139:LEU:HD23	1.99	0.45
1:BBB:325:GLY:O	1:BBB:462:THR:HA	2.16	0.45
1:AAA:418:THR:OG1	1:AAA:425:GLU:OE2	2.33	0.44
1:AAA:411:LYS:HB3	1:AAA:505:ILE:HG21	1.99	0.44
1:AAA:107:ARG:HA	1:AAA:112:LEU:HB3	1.99	0.44
1:AAA:587:ILE:HG12	1:AAA:598:VAL:HG23	1.98	0.44
1:BBB:174:THR:O	1:BBB:178:GLY:HA2	2.18	0.44
1:AAA:386:GLU:HG2	1:AAA:522:GLY:HA3	2.00	0.44
1:BBB:573:VAL:HA	1:BBB:585:VAL:O	2.18	0.44
1:BBB:587:ILE:HG12	1:BBB:598:VAL:HG23	2.00	0.44
1:BBB:538:THR:HG22	1:BBB:603:ARG:CZ	2.48	0.44
1:AAA:325:GLY:O	1:AAA:462:THR:HA	2.17	0.44
1:BBB:173:LEU:HD23	1:BBB:260:GLN:HG2	1.99	0.44
1:BBB:273:ALA:HA	1:BBB:288:VAL:O	2.17	0.43
1:AAA:534:PHE:O	1:AAA:603:ARG:CG	2.66	0.43
1:AAA:573:VAL:HA	1:AAA:585:VAL:O	2.18	0.43
1:BBB:210:GLY:HA2	1:BBB:422:LEU:HD22	2.00	0.43
1:AAA:79:PRO:HB3	1:AAA:82:LEU:HD21	2.00	0.43
1:AAA:89:LEU:HB3	1:AAA:135:VAL:HG13	2.00	0.43
1:AAA:210:GLY:HA2	1:AAA:422:LEU:HD22	2.00	0.43
1:AAA:197:LEU:N	1:AAA:198:PRO:CD	2.82	0.43
1:AAA:329:PRO:HB2	1:AAA:333:VAL:HG13	2.00	0.43
1:BBB:89:LEU:O	1:BBB:135:VAL:N	2.46	0.43
1:BBB:290:ASN:ND2	1:BBB:291:PRO:HA	2.34	0.43
1:AAA:437:GLN:O	1:AAA:441:LYS:HA	2.19	0.42
1:BBB:386:GLU:HG2	1:BBB:522:GLY:HA3	2.02	0.42
1:AAA:176:VAL:CG2	1:AAA:255:LEU:HD11	2.49	0.42
1:BBB:197:LEU:N	1:BBB:198:PRO:CD	2.82	0.42
1:AAA:330:ALA:N	1:AAA:455:GLY:O	2.50	0.42
1:AAA:73:PHE:CD2	1:AAA:252:TYR:CE1	3.08	0.42
1:AAA:420:ILE:HA	1:AAA:482:PRO:O	2.20	0.42
1:AAA:89:LEU:HA	1:AAA:89:LEU:HD23	1.86	0.42
1:AAA:200:TYR:CZ	1:AAA:220:HIS:ND1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:270:SER:HB3	1:AAA:594:ALA:CB	2.49	0.41
1:BBB:257:LEU:O	1:BBB:261:ILE:HG12	2.20	0.41
1:BBB:400:MET:O	1:BBB:404:ARG:HG2	2.21	0.41
1:BBB:429:LEU:HD11	1:BBB:435:TRP:NE1	2.36	0.41
1:AAA:330:ALA:O	1:AAA:333:VAL:HG22	2.20	0.41
1:BBB:197:LEU:N	1:BBB:198:PRO:HD2	2.36	0.41
1:BBB:343:SER:HA	1:BBB:512:TYR:HE2	1.84	0.41
1:BBB:437:GLN:O	1:BBB:441:LYS:HA	2.21	0.41
1:BBB:485:LEU:HD23	1:BBB:497:TYR:CD1	2.56	0.41
1:BBB:121:GLU:HA	1:BBB:124:ARG:HG3	2.01	0.41
1:BBB:302:ILE:HG21	1:BBB:307:TYR:HB2	2.02	0.41
1:AAA:207:GLY:N	1:AAA:216:GLU:OE1	2.35	0.41
1:BBB:503:THR:HG22	1:BBB:504:GLN:H	1.86	0.41
1:BBB:327:TYR:CD2	1:BBB:588:ILE:HD13	2.55	0.41
1:BBB:333:VAL:HG13	1:BBB:337:ILE:HG13	2.03	0.41
1:BBB:89:LEU:HB3	1:BBB:135:VAL:HG13	2.02	0.41
1:AAA:327:TYR:CD2	1:AAA:588:ILE:HD13	2.57	0.40
1:BBB:262:TYR:CD2	1:BBB:608:HIS:CD2	3.09	0.40
1:BBB:333:VAL:HG22	1:BBB:459:TRP:CH2	2.56	0.40
1:BBB:408:TRP:O	1:BBB:411:LYS:HB2	2.20	0.40
1:AAA:355:ASP:OD1	1:AAA:357:GLY:N	2.40	0.40
1:AAA:421:ASP:OD1	1:AAA:421:ASP:N	2.49	0.40
1:BBB:330:ALA:N	1:BBB:455:GLY:O	2.50	0.40
1:BBB:572:MET:HE2	1:BBB:602:THR:HB	2.03	0.40
1:BBB:86:ILE:HG23	1:BBB:138:PRO:HB3	2.02	0.40
1:AAA:183:ILE:HG23	1:AAA:187:ASP:HB2	2.03	0.40
1:AAA:294:ASP:HB3	1:AAA:297:LEU:HG	2.03	0.40
1:AAA:360:GLN:HA	1:AAA:367:ARG:HA	2.03	0.40
1:BBB:150:ASN:N	1:BBB:150:ASN:ND2	2.69	0.40
1:BBB:316:ARG:O	1:BBB:319:ILE:HG22	2.22	0.40
1:BBB:420:ILE:HA	1:BBB:482:PRO:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AAA	486/583 (83%)	454 (93%)	31 (6%)	1 (0%)	47 78
1	BBB	523/583 (90%)	487 (93%)	35 (7%)	1 (0%)	47 78
All	All	1009/1166 (86%)	941 (93%)	66 (6%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	595	GLY
1	BBB	595	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
1	AAA	415/494 (84%)	383 (92%)	32 (8%)	13 35
1	BBB	450/494 (91%)	408 (91%)	42 (9%)	9 26
All	All	865/988 (88%)	791 (91%)	74 (9%)	10 30

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	75	ARG
1	AAA	89	LEU
1	AAA	99	LEU
1	AAA	102	THR
1	AAA	114	ASP
1	AAA	140	THR
1	AAA	150	ASN
1	AAA	218	THR
1	AAA	246	GLN
1	AAA	249	LYS
1	AAA	251	ILE

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Mol	Chain	Res	Type
1	AAA	255	LEU
1	AAA	290	ASN
1	AAA	300	ASP
1	AAA	302	ILE
1	AAA	303	SER
1	AAA	308	GLN
1	AAA	311	LEU
1	AAA	315	ASN
1	AAA	381	VAL
1	AAA	421	ASP
1	AAA	456	GLN
1	AAA	478	THR
1	AAA	495	VAL
1	AAA	502	SER
1	AAA	505	ILE
1	AAA	508	ILE
1	AAA	530	THR
1	AAA	532	ARG
1	AAA	545	LYS
1	AAA	579	GLU
1	AAA	603	ARG
1	BBB	62	LEU
1	BBB	75	ARG
1	BBB	92	MET
1	BBB	94	GLU
1	BBB	99	LEU
1	BBB	114	ASP
1	BBB	124	ARG
1	BBB	127	SER
1	BBB	136	LYS
1	BBB	140	THR
1	BBB	150	ASN
1	BBB	184	ASN
1	BBB	218	THR
1	BBB	238	ARG
1	BBB	255	LEU
1	BBB	290	ASN
1	BBB	300	ASP
1	BBB	302	ILE
1	BBB	308	GLN
1	BBB	315	ASN
1	BBB	316	ARG

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Mol	Chain	Res	Type
1	BBB	333	VAL
1	BBB	360	GLN
1	BBB	367	ARG
1	BBB	369	ARG
1	BBB	381	VAL
1	BBB	421	ASP
1	BBB	429	LEU
1	BBB	456	GLN
1	BBB	478	THR
1	BBB	495	VAL
1	BBB	499	GLN
1	BBB	501	ASP
1	BBB	503	THR
1	BBB	530	THR
1	BBB	532	ARG
1	BBB	545	LYS
1	BBB	567	ARG
1	BBB	572	MET
1	BBB	579	GLU
1	BBB	580	ASN
1	BBB	588	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DH4	BBB	701	1	15,23,23	0.28	0	14,32,32	0.71	0
2	DH4	AAA	701	1	15,23,23	0.28	0	14,32,32	0.69	0

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
2	DH4	BBB	701	1	-	2/2/39/39	0/2/2/2
2	DH4	AAA	701	1	-	2/2/39/39	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	701	DH4	C6-CA-N-CAC
2	BBB	701	DH4	NAL-CAC-N-CA
2	AAA	701	DH4	C6-CA-N-CAC
2	AAA	701	DH4	NAL-CAC-N-CA

There are no ring outliers.

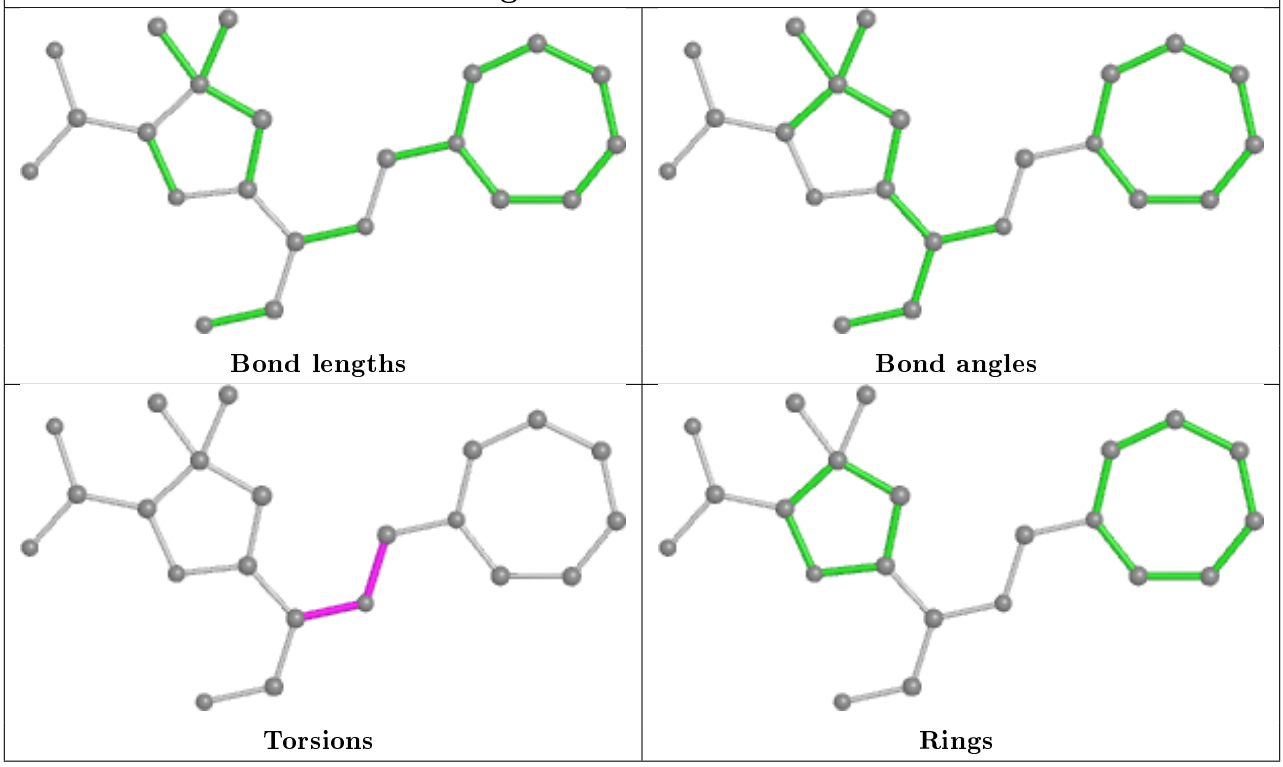
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	701	DH4	1	0
2	AAA	701	DH4	2	0

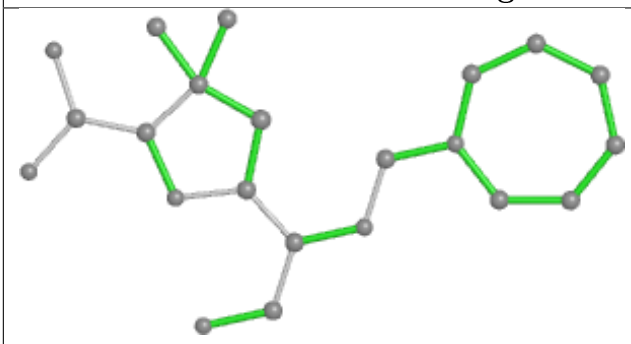
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

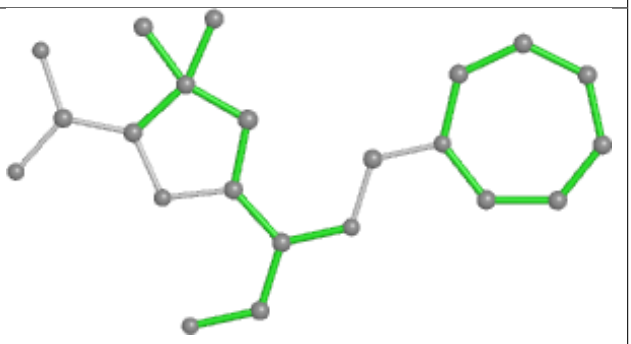
Ligand DH4 BBB 701



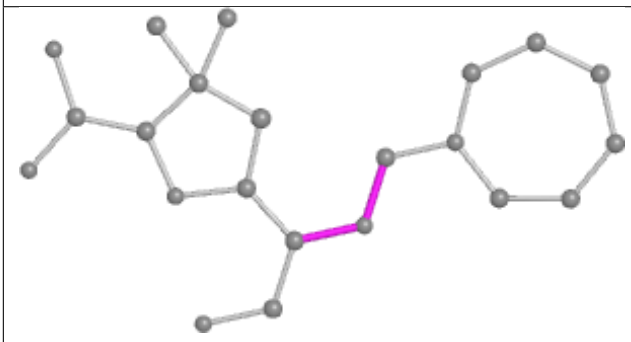
Ligand DH4 AAA 701



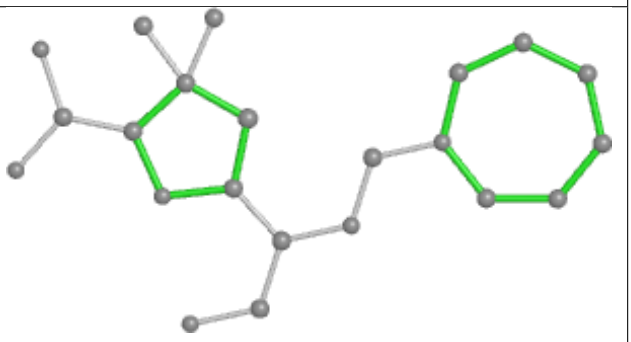
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	AAA	498/583 (85%)	0.04	17 (3%) 45 35	40, 67, 105, 132	0
1	BBB	533/583 (91%)	-0.10	4 (0%) 86 81	40, 68, 105, 137	0
All	All	1031/1166 (88%)	-0.03	21 (2%) 65 56	40, 68, 105, 137	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	193	LYS	4.1
1	BBB	131	THR	3.7
1	AAA	189	GLU	3.7
1	AAA	103	LEU	3.5
1	AAA	135	VAL	3.3
1	BBB	233	ARG	3.3
1	AAA	593	GLY	3.0
1	AAA	134	ALA	2.9
1	AAA	119	ASN	2.9
1	AAA	117	ILE	2.9
1	AAA	133	ILE	2.8
1	AAA	156	GLY	2.6
1	BBB	93	PRO	2.6
1	AAA	542	ALA	2.6
1	AAA	187	ASP	2.4
1	AAA	184	ASN	2.4
1	AAA	182	LYS	2.3
1	BBB	352	SER	2.2
1	AAA	611	LEU	2.2
1	AAA	155	PRO	2.1
1	AAA	90	GLU	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)

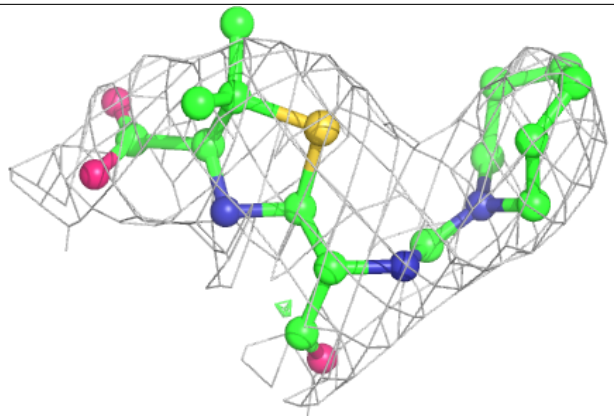
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

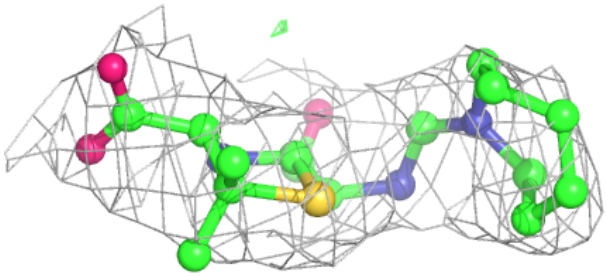
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DH4	BBB	701	22/22	0.94	0.17	75,90,92,93	0
2	DH4	AAA	701	22/22	0.94	0.17	74,85,91,91	0

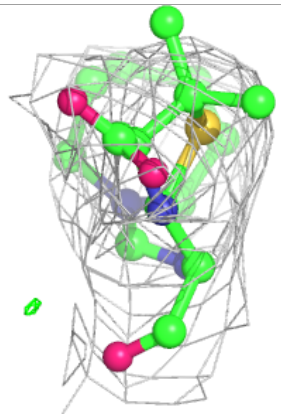
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DH4 BBB 701:

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

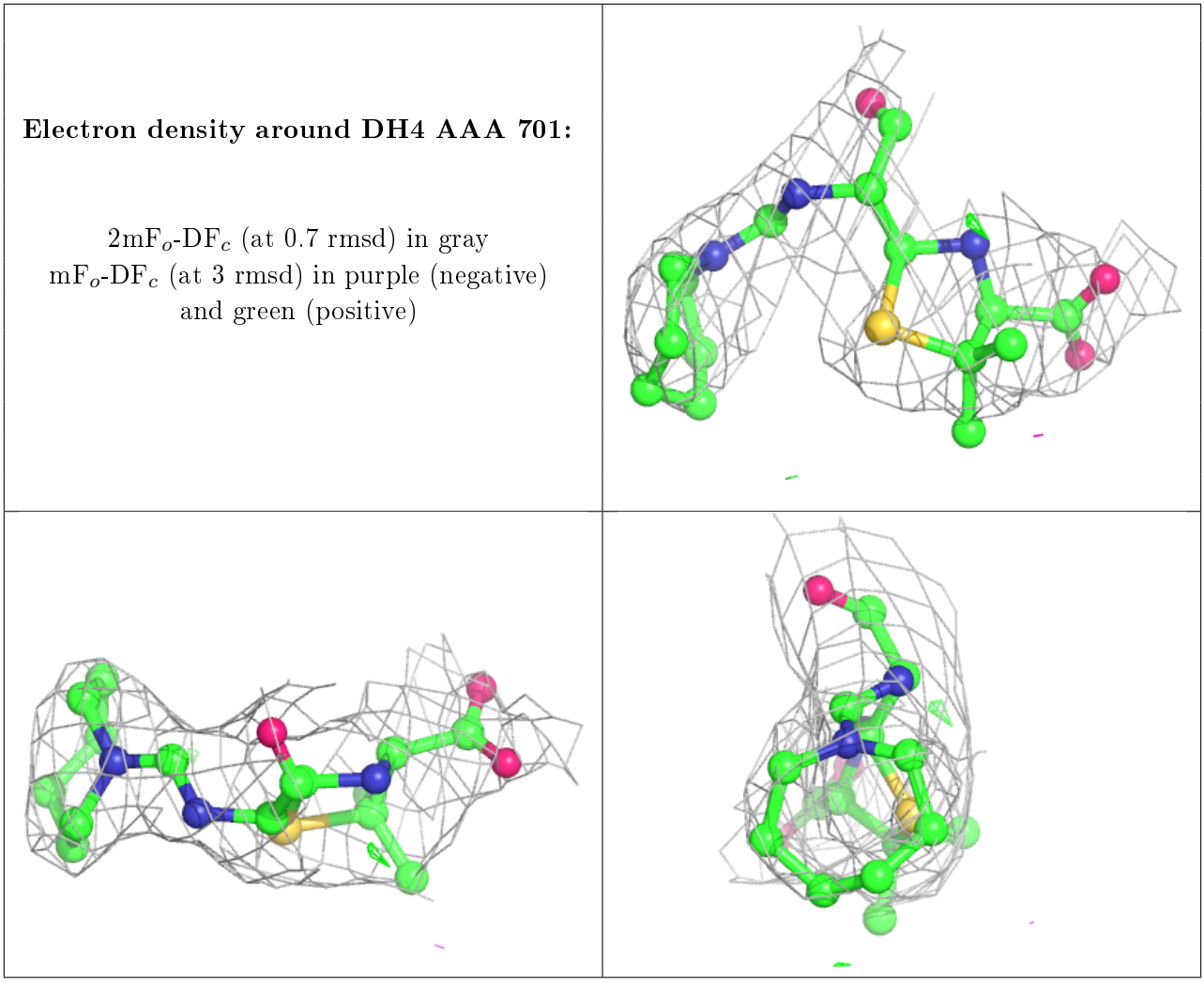






Electron density around DH4 AAA 701:

$2mF_o$-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

There are no such residues in this entry.