



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2021 – 12:04 am BST

PDB ID : 6ZIC  
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE-1 (RPMFE1) COMPLEXED WITH 3S-HYDROXYBUTANOYL-COA AND NADH  
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Deposited on : 2020-06-25  
Resolution : 2.20 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](mailto: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.

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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 : 2.22  
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) : 2.22

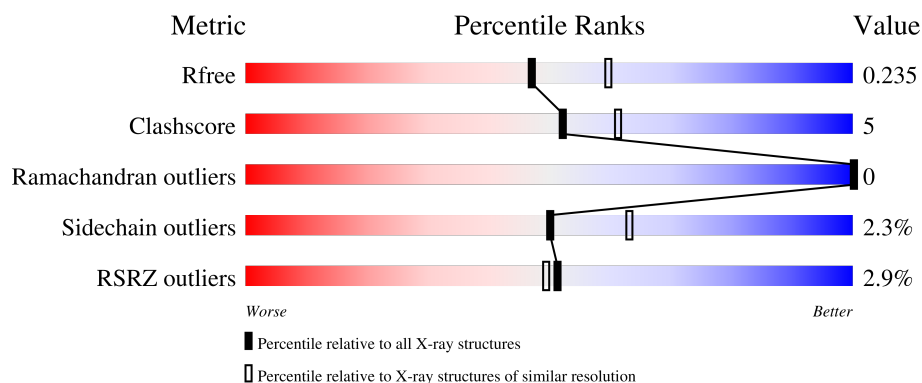
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	742	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	BBB	742	<div> <div>4%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11611 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 Peroxisomal bifunctional enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	723	Total	C	N	O	S	0	4	0
			5589	3567	986	1013	23			
1	BBB	714	Total	C	N	O	S	0	3	0
			5519	3529	967	1000	23			

There are 40 discrepancies between the modelled and reference sequences:

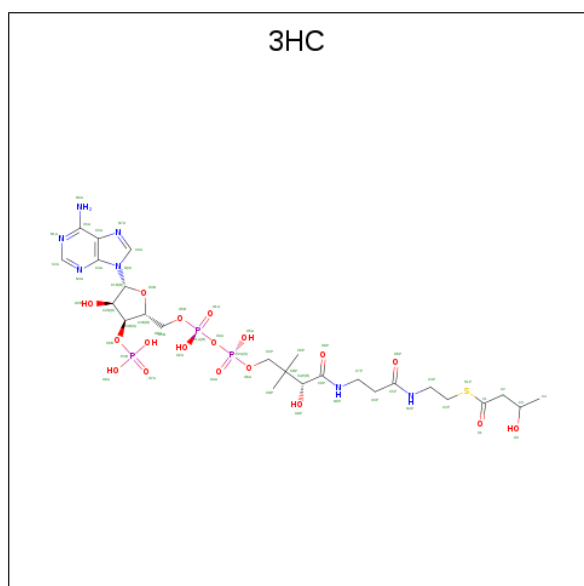
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP P07896
AAA	-18	GLY	-	expression tag	UNP P07896
AAA	-17	SER	-	expression tag	UNP P07896
AAA	-16	SER	-	expression tag	UNP P07896
AAA	-15	HIS	-	expression tag	UNP P07896
AAA	-14	HIS	-	expression tag	UNP P07896
AAA	-13	HIS	-	expression tag	UNP P07896
AAA	-12	HIS	-	expression tag	UNP P07896
AAA	-11	HIS	-	expression tag	UNP P07896
AAA	-10	HIS	-	expression tag	UNP P07896
AAA	-9	SER	-	expression tag	UNP P07896
AAA	-8	SER	-	expression tag	UNP P07896
AAA	-7	GLY	-	expression tag	UNP P07896
AAA	-6	LEU	-	expression tag	UNP P07896
AAA	-5	VAL	-	expression tag	UNP P07896
AAA	-4	PRO	-	expression tag	UNP P07896
AAA	-3	ARG	-	expression tag	UNP P07896
AAA	-2	GLY	-	expression tag	UNP P07896
AAA	-1	SER	-	expression tag	UNP P07896
AAA	0	HIS	-	expression tag	UNP P07896
BBB	-19	MET	-	initiating methionine	UNP P07896
BBB	-18	GLY	-	expression tag	UNP P07896
BBB	-17	SER	-	expression tag	UNP P07896
BBB	-16	SER	-	expression tag	UNP P07896
BBB	-15	HIS	-	expression tag	UNP P07896

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-14	HIS	-	expression tag	UNP P07896
BBB	-13	HIS	-	expression tag	UNP P07896
BBB	-12	HIS	-	expression tag	UNP P07896
BBB	-11	HIS	-	expression tag	UNP P07896
BBB	-10	HIS	-	expression tag	UNP P07896
BBB	-9	SER	-	expression tag	UNP P07896
BBB	-8	SER	-	expression tag	UNP P07896
BBB	-7	GLY	-	expression tag	UNP P07896
BBB	-6	LEU	-	expression tag	UNP P07896
BBB	-5	VAL	-	expression tag	UNP P07896
BBB	-4	PRO	-	expression tag	UNP P07896
BBB	-3	ARG	-	expression tag	UNP P07896
BBB	-2	GLY	-	expression tag	UNP P07896
BBB	-1	SER	-	expression tag	UNP P07896
BBB	0	HIS	-	expression tag	UNP P07896

- Molecule 2 is 3-HYDROXYBUTANOYL-COENZYME A (three-letter code: 3HC) (formula:  $C_{25}H_{42}N_7O_{18}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



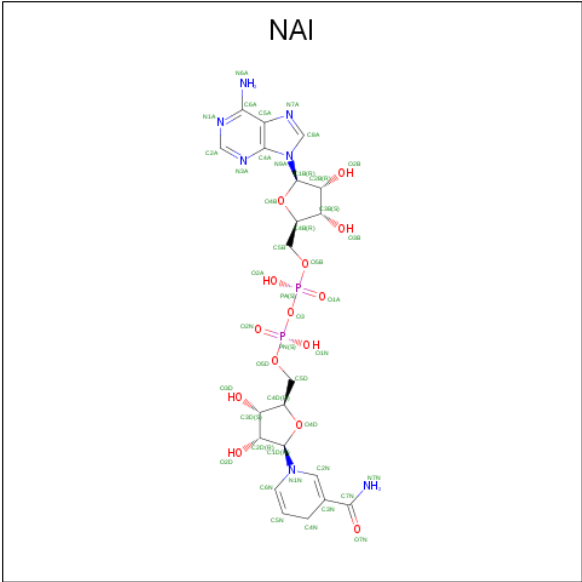
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	BBB	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



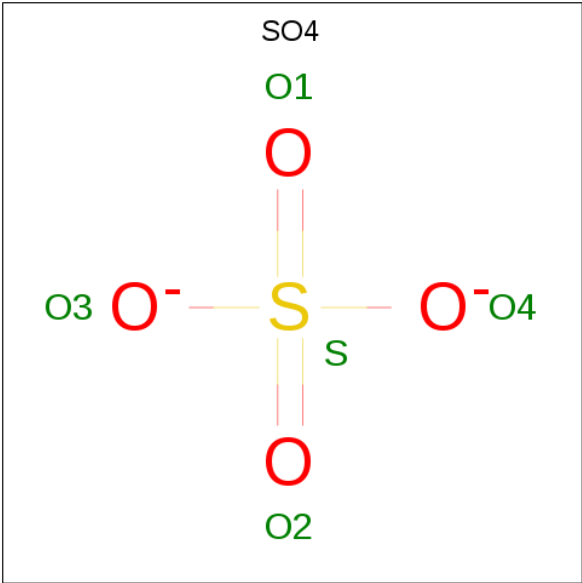
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	BBB	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		

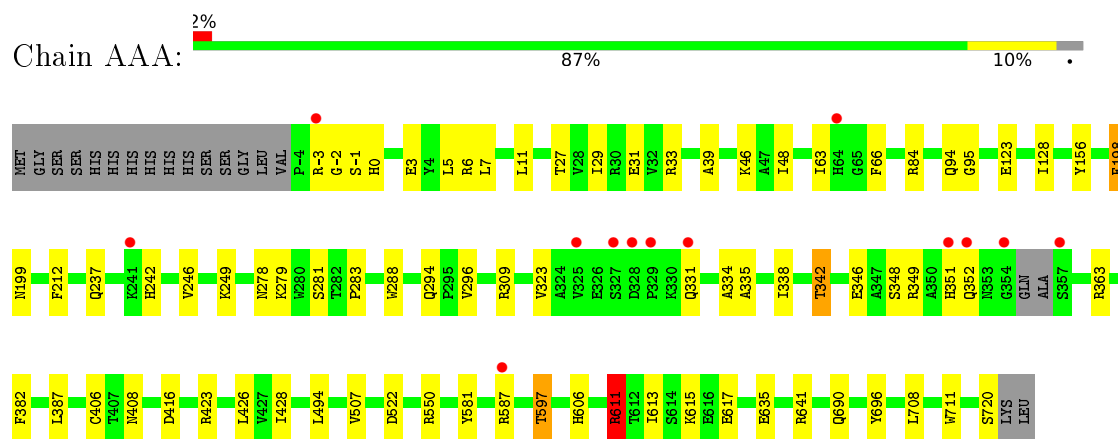
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	187	Total 187	O 187	0	0
6	BBB	68	Total 68	O 68	0	0

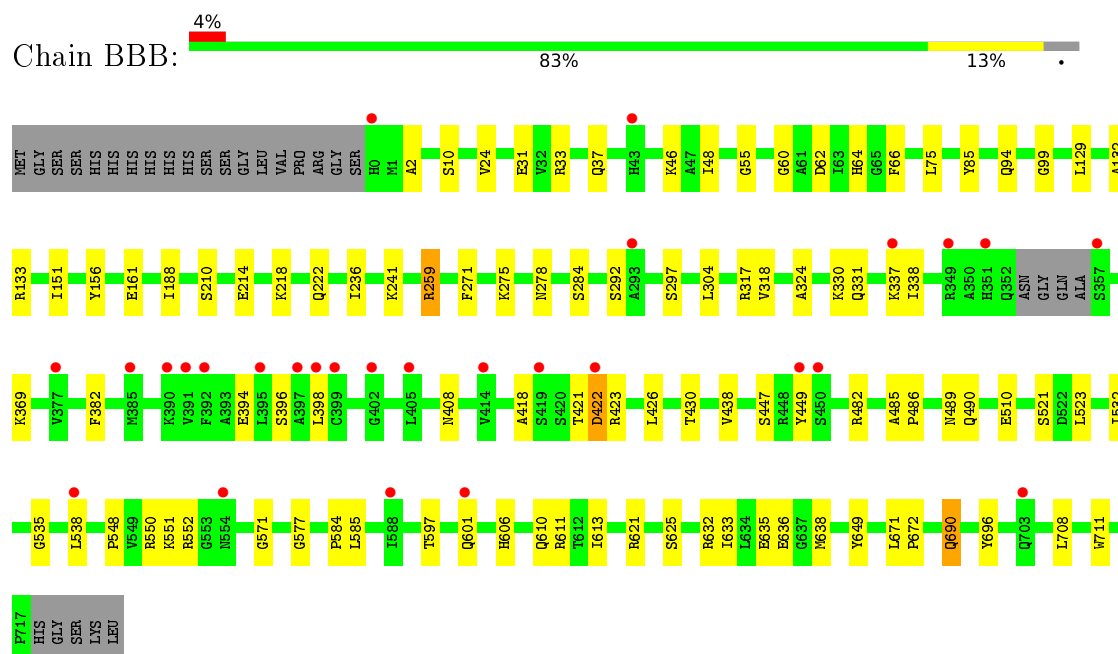
### 3 Residue-property plots [i](#)

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: Peroxisomal bifunctional enzyme



- Molecule 1: Peroxisomal bifunctional enzyme





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.64Å 127.09Å 227.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.12 – 2.20 65.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (65.12-2.20) 99.5 (65.04-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.200 , 0.234 0.204 , 0.235	Depositor DCC
$R_{free}$ test set	4925 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11611	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 3HC, GOL, NAI

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	0.48	0/5717	0.82	3/7740 (0.0%)
1	BBB	0.41	1/5645 (0.0%)	0.74	4/7645 (0.1%)
All	All	0.44	1/11362 (0.0%)	0.78	7/15385 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	538	LEU	C-O	5.80	1.34	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	278	ASN	CB-CA-C	-10.52	89.36	110.40
1	BBB	611	ARG	CB-CG-CD	-6.70	94.18	111.60
1	AAA	611	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	BBB	278	ASN	CB-CA-C	-5.50	99.41	110.40
1	BBB	649	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	AAA	294	GLN	CB-CA-C	-5.25	99.91	110.40
1	BBB	259	ARG	CB-CG-CD	-5.00	98.59	111.60

There are no chirality outliers.

There are no planarity outliers.

### 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	AAA	5589	0	5692	62	0
1	BBB	5519	0	5630	61	0
2	AAA	54	0	38	7	0
2	BBB	54	0	38	3	0
3	AAA	36	0	48	10	0
3	BBB	6	0	8	1	0
4	AAA	44	0	27	6	0
4	BBB	44	0	27	3	0
5	AAA	5	0	0	0	0
5	BBB	5	0	0	0	0
6	AAA	187	0	0	2	0
6	BBB	68	0	0	1	0
All	All	11611	0	11508	125	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 5.

All (125) 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:BBB:46:LYS:HB2	1:BBB:188:ILE:HD11	1.54	0.90
1:BBB:46:LYS:CB	1:BBB:188:ILE:HD11	2.05	0.86
1:AAA:641:ARG:HH12	3:AAA:805:GOL:H32	1.43	0.82
1:AAA:288:TRP:HE1	3:AAA:803:GOL:H11	1.45	0.81
1:AAA:296:VAL:H	3:AAA:808:GOL:H11	1.48	0.79
1:BBB:635:GLU:HB2	6:BBB:934:HOH:O	1.83	0.79
3:AAA:802:GOL:H11	6:AAA:956:HOH:O	1.87	0.75
1:AAA:63:ILE:HG13	2:AAA:801:3HC:C6A	2.16	0.75
1:AAA:720:SER:C	3:AAA:807:GOL:O2	2.24	0.74
1:AAA:-1:SER:N	1:AAA:31:GLU:OE2	2.23	0.72
1:AAA:597:THR:HG23	1:BBB:382:PHE:CZ	2.26	0.71
1:BBB:635:GLU:HB3	1:BBB:696:TYR:HB2	1.72	0.70
1:BBB:396:SER:OG	1:BBB:422:ASP:HB2	1.92	0.70
1:AAA:309:ARG:NH1	1:AAA:335:ALA:HB2	2.07	0.69
1:AAA:123:GLU:CG	2:AAA:801:3HC:HC22	2.22	0.68
1:AAA:63:ILE:HG13	2:AAA:801:3HC:N6A	2.09	0.67
1:AAA:281:SER:O	3:AAA:802:GOL:H2	1.96	0.65
1:AAA:611:ARG:NH2	1:AAA:617:GLU:OE1	2.30	0.64
1:AAA:283:PRO:HD3	3:AAA:802:GOL:H32	1.81	0.63
1:BBB:369:LYS:HA	1:BBB:398:LEU:CD1	2.29	0.62
1:BBB:490:GLN:NE2	1:BBB:621:ARG:HE	1.98	0.62
1:AAA:641:ARG:NH1	3:AAA:805:GOL:H32	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:309:ARG:HD3	1:AAA:338:ILE:HG21	1.84	0.59
1:BBB:46:LYS:HB3	1:BBB:188:ILE:HD11	1.82	0.59
1:BBB:60:GLY:HA3	2:BBB:801:3HC:H31	1.85	0.59
1:BBB:369:LYS:HA	1:BBB:398:LEU:HD12	1.85	0.58
1:AAA:309:ARG:HH11	1:AAA:335:ALA:HB2	1.69	0.57
1:BBB:597:THR:O	1:BBB:601:GLN:HG3	2.04	0.57
1:BBB:369:LYS:HD2	1:BBB:398:LEU:HD12	1.87	0.57
1:BBB:625:SER:HB2	1:BBB:690:GLN:HE22	1.69	0.57
1:AAA:123:GLU:HG2	2:AAA:801:3HC:HC22	1.85	0.57
1:AAA:-2:GLY:HA2	1:AAA:31:GLU:OE2	2.06	0.56
1:BBB:632:ARG:HA	1:BBB:635:GLU:HG2	1.87	0.56
1:AAA:342:THR:O	1:AAA:346:GLU:HG3	2.06	0.55
1:AAA:611:ARG:HH22	1:AAA:617:GLU:CD	2.09	0.55
1:BBB:218:LYS:HG3	1:BBB:222:GLN:HE21	1.71	0.55
1:AAA:338:ILE:O	1:AAA:342:THR:HG23	2.06	0.55
1:AAA:597:THR:HG23	1:BBB:382:PHE:CE1	2.42	0.55
1:AAA:331:GLN:HG2	4:AAA:806:NAI:O3B	2.07	0.55
1:BBB:550:ARG:HD2	1:BBB:606:HIS:CG	2.43	0.54
1:BBB:66:PHE:HZ	2:BBB:801:3HC:S1P	2.30	0.54
1:BBB:151:ILE:HD12	1:BBB:236:ILE:HD11	1.88	0.54
1:BBB:532:ILE:O	1:BBB:535:GLY:N	2.40	0.54
1:AAA:597:THR:HG23	1:BBB:382:PHE:HZ	1.71	0.54
1:AAA:348:SER:HA	1:AAA:351:HIS:HB2	1.90	0.54
1:BBB:394:GLU:O	1:BBB:398:LEU:HD22	2.08	0.53
1:AAA:309:ARG:HD3	1:AAA:338:ILE:CG2	2.39	0.53
1:AAA:387:LEU:HD11	4:AAA:806:NAI:H61A	1.74	0.52
1:BBB:55:GLY:HA2	1:BBB:94:GLN:HG2	1.91	0.52
1:BBB:218:LYS:HE3	1:BBB:222:GLN:HE22	1.74	0.52
1:BBB:24:VAL:HG11	1:BBB:75:LEU:HD13	1.92	0.51
1:BBB:408:ASN:HA	1:BBB:430:THR:O	2.10	0.51
1:BBB:210:SER:O	1:BBB:214:GLU:HB3	2.12	0.50
1:AAA:29:ILE:O	1:AAA:33[A]:ARG:HG3	2.12	0.50
1:BBB:62:ASP:OD1	1:BBB:64:HIS:HB2	2.11	0.49
1:AAA:309:ARG:HH11	1:AAA:335:ALA:CB	2.25	0.49
1:AAA:406:CYS:HA	1:AAA:428:ILE:O	2.13	0.49
3:AAA:803:GOL:O3	3:AAA:803:GOL:O1	2.29	0.49
1:AAA:708:LEU:C	1:AAA:708:LEU:HD23	2.33	0.48
3:BBB:802:GOL:O1	3:BBB:802:GOL:O3	2.22	0.48
1:AAA:84[A]:ARG:NH2	6:AAA:901:HOH:O	2.19	0.48
1:AAA:94:GLN:HG3	1:AAA:95:GLY:N	2.27	0.48
1:BBB:304:LEU:HD11	1:BBB:324:ALA:HB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:63:ILE:HD11	2:AAA:801:3HC:C5P	2.43	0.48
1:AAA:494:LEU:HD22	1:AAA:613:ILE:HG21	1.96	0.48
1:BBB:382:PHE:CE2	4:BBB:803:NAI:H8A	2.49	0.48
1:BBB:584:PRO:O	1:BBB:585:LEU:HB2	2.14	0.48
1:AAA:63:ILE:HA	1:AAA:66:PHE:CD1	2.49	0.47
1:AAA:587:ARG:HE	1:AAA:587:ARG:HB3	1.54	0.47
1:BBB:423:ARG:HB2	1:BBB:426:LEU:HD12	1.96	0.47
1:AAA:334:ALA:O	1:AAA:338:ILE:HG22	2.15	0.47
1:BBB:129:LEU:HD12	1:BBB:129:LEU:C	2.35	0.47
1:AAA:63:ILE:CG1	2:AAA:801:3HC:N6A	2.77	0.46
1:AAA:323:VAL:HG22	1:AAA:363:ARG:NH1	2.30	0.46
1:AAA:242:HIS:HB3	1:AAA:246:VAL:HB	1.96	0.46
1:AAA:550:ARG:HD2	1:AAA:606:HIS:CG	2.50	0.46
1:BBB:369:LYS:HA	1:BBB:398:LEU:HD11	1.96	0.46
1:AAA:309:ARG:NH1	1:AAA:335:ALA:CB	2.79	0.46
1:BBB:10:SER:HB3	1:BBB:46:LYS:HG3	1.97	0.46
1:AAA:156:TYR:N	1:AAA:156:TYR:CD1	2.84	0.46
1:BBB:548:PRO:HG2	1:BBB:551:LYS:HB3	1.97	0.45
1:BBB:33[B]:ARG:O	1:BBB:37:GLN:HG3	2.16	0.45
1:AAA:507:VAL:HG22	1:AAA:615:LYS:HE3	1.99	0.45
1:BBB:156:TYR:N	1:BBB:156:TYR:CD1	2.85	0.44
1:AAA:382:PHE:CE1	4:AAA:806:NAI:H3B	2.52	0.44
1:BBB:671:LEU:N	1:BBB:672:PRO:CD	2.79	0.44
1:AAA:7:LEU:HB2	1:AAA:11:LEU:HB2	2.00	0.44
1:BBB:482:ARG:HH22	1:BBB:636:GLU:CD	2.21	0.43
1:AAA:423:ARG:HB2	1:AAA:426:LEU:HD12	2.00	0.43
1:BBB:317:ARG:HG3	1:BBB:318:VAL:HG13	2.00	0.43
1:AAA:279:LYS:NZ	3:AAA:805:GOL:H2	2.33	0.43
1:AAA:198:PHE:HD1	1:AAA:199:ASN:N	2.17	0.43
1:BBB:271:PHE:O	1:BBB:275:LYS:HG2	2.18	0.43
1:BBB:2:ALA:HB3	1:BBB:31:GLU:HB3	2.01	0.43
1:BBB:382:PHE:CZ	4:BBB:803:NAI:H2B	2.54	0.43
1:AAA:349:ARG:O	1:AAA:352:GLN:HB2	2.19	0.43
1:BBB:48:ILE:HD12	1:BBB:85:TYR:CE2	2.55	0.42
1:BBB:490:GLN:HE22	1:BBB:621:ARG:HH21	1.66	0.42
4:AAA:806:NAI:O1N	4:AAA:806:NAI:N7N	2.52	0.42
1:BBB:551:LYS:O	1:BBB:552:ARG:NH1	2.44	0.42
1:AAA:522:ASP:OD2	1:AAA:581:TYR:OH	2.33	0.42
1:BBB:331:GLN:HG2	4:BBB:803:NAI:O3B	2.19	0.42
1:BBB:708:LEU:HA	1:BBB:711:TRP:CE2	2.54	0.42
1:AAA:123:GLU:HG3	2:AAA:801:3HC:HC22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:212:PHE:CZ	1:AAA:237:GLN:HA	2.55	0.42
1:BBB:156:TYR:N	1:BBB:156:TYR:HD1	2.18	0.41
1:AAA:-3:ARG:HD3	1:AAA:27:THR:OG1	2.21	0.41
1:BBB:571:GLY:HA2	1:BBB:577:GLY:HA3	2.02	0.41
1:AAA:708:LEU:HA	1:AAA:711:TRP:CE2	2.55	0.41
1:BBB:486:PRO:HA	1:BBB:489:ASN:HB2	2.02	0.41
1:AAA:635:GLU:HB3	1:AAA:696:TYR:HB2	2.03	0.41
4:AAA:806:NAI:H2N	4:AAA:806:NAI:H2D	1.85	0.41
1:AAA:123:GLU:HB3	1:AAA:128:ILE:HG13	2.03	0.41
1:BBB:625:SER:HB2	1:BBB:690:GLN:NE2	2.33	0.41
1:AAA:39:ALA:HB3	1:AAA:48:ILE:HD11	2.02	0.41
1:BBB:418:ALA:O	1:BBB:421:THR:OG1	2.37	0.40
1:BBB:447:SER:C	1:BBB:449:TYR:H	2.25	0.40
1:AAA:309:ARG:NH1	1:AAA:335:ALA:CA	2.84	0.40
1:BBB:99:GLY:HA3	2:BBB:801:3HC:H22	2.03	0.40
1:BBB:218:LYS:HE3	1:BBB:222:GLN:NE2	2.35	0.40
1:AAA:0:HIS:HD2	1:AAA:3:GLU:OE1	2.04	0.40
1:BBB:132:ALA:O	1:BBB:133:ARG:HB2	2.22	0.40
1:BBB:633:ILE:HG23	1:BBB:638:MET:HB2	2.02	0.40
1:AAA:408:ASN:O	4:AAA:806:NAI:H1D	2.22	0.40
1:BBB:485:ALA:N	1:BBB:486:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	723/742 (97%)	698 (96%)	25 (4%)	0	100	100
1	BBB	713/742 (96%)	683 (96%)	30 (4%)	0	100	100
All	All	1436/1484 (97%)	1381 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	597/609 (98%)	587 (98%)	10 (2%)	60	74
1	BBB	590/609 (97%)	573 (97%)	17 (3%)	42	54
All	All	1187/1218 (98%)	1160 (98%)	27 (2%)	50	63

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	5	LEU
1	AAA	6	ARG
1	AAA	46	LYS
1	AAA	198	PHE
1	AAA	249	LYS
1	AAA	342	THR
1	AAA	416	ASP
1	AAA	597	THR
1	AAA	611	ARG
1	AAA	690	GLN
1	BBB	161	GLU
1	BBB	241	LYS
1	BBB	259	ARG
1	BBB	284	SER
1	BBB	292	SER
1	BBB	297	SER
1	BBB	330	LYS
1	BBB	337	LYS
1	BBB	338	ILE
1	BBB	422	ASP
1	BBB	438	VAL
1	BBB	510	GLU
1	BBB	521	SER
1	BBB	523	LEU
1	BBB	610	GLN

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Mol	Chain	Res	Type
1	BBB	613	ILE
1	BBB	690	GLN

Sometimes 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 ⓘ

13 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	$\# Z  > 2$
3	GOL	AAA	807	-	5,5,5	0.13	0	5,5,5	0.37	0
2	3HC	AAA	801	-	47,56,56	0.57	0	59,83,83	0.83	3 (5%)
3	GOL	AAA	808	-	5,5,5	0.10	0	5,5,5	0.33	0
3	GOL	AAA	802	-	5,5,5	0.12	0	5,5,5	0.50	0
4	NAI	AAA	806	-	42,48,48	0.60	0	47,73,73	0.94	3 (6%)
3	GOL	AAA	804	-	5,5,5	0.13	0	5,5,5	0.42	0
3	GOL	BBB	802	-	5,5,5	0.10	0	5,5,5	0.30	0
2	3HC	BBB	801	-	47,56,56	0.54	0	59,83,83	0.66	1 (1%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	AAA	809	-	4,4,4	0.29	0	6,6,6	0.20	0
5	SO4	BBB	804	-	4,4,4	0.37	0	6,6,6	0.08	0
3	GOL	AAA	803	-	5,5,5	0.13	0	5,5,5	0.60	0
3	GOL	AAA	805	-	5,5,5	0.09	0	5,5,5	0.55	0
4	NAI	BBB	803	-	42,48,48	0.59	0	47,73,73	0.67	1 (2%)

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
3	GOL	AAA	807	-	-	0/4/4/4	-
2	3HC	AAA	801	-	-	22/51/71/71	0/3/3/3
3	GOL	AAA	808	-	-	2/4/4/4	-
3	GOL	AAA	802	-	-	2/4/4/4	-
4	NAI	AAA	806	-	-	10/25/72/72	0/5/5/5
3	GOL	AAA	804	-	-	2/4/4/4	-
3	GOL	BBB	802	-	-	2/4/4/4	-
2	3HC	BBB	801	-	-	14/51/71/71	0/3/3/3
3	GOL	AAA	803	-	-	4/4/4/4	-
3	GOL	AAA	805	-	-	4/4/4/4	-
4	NAI	BBB	803	-	-	5/25/72/72	0/5/5/5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	806	NAI	C5A-C6A-N6A	2.55	124.23	120.35
2	AAA	801	3HC	C3B-C2B-C1B	2.54	105.52	99.89
2	AAA	801	3HC	C5A-C6A-N6A	2.32	123.88	120.35
4	AAA	806	NAI	C3B-C2B-C1B	2.19	104.28	100.98
2	AAA	801	3HC	C7P-C6P-C5P	-2.17	108.74	112.36
4	BBB	803	NAI	C5A-C6A-N6A	2.16	123.64	120.35
2	BBB	801	3HC	C5A-C6A-N6A	2.16	123.63	120.35
4	AAA	806	NAI	O2A-PA-O1A	2.11	122.67	112.24

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	801	3HC	P1A-O3A-P2A-O6A
2	AAA	801	3HC	CCP-O6A-P2A-O4A
2	AAA	801	3HC	CCP-O6A-P2A-O5A
2	AAA	801	3HC	O9P-C9P-CAP-CBP
2	AAA	801	3HC	N8P-C9P-CAP-CBP
2	AAA	801	3HC	N8P-C9P-CAP-OAP
2	AAA	801	3HC	CAP-C9P-N8P-C7P
2	AAA	801	3HC	C5P-C6P-C7P-N8P
2	AAA	801	3HC	C1-C2-C3-O3
2	AAA	801	3HC	C1-C2-C3-C4
2	BBB	801	3HC	C3B-O3B-P3B-O8A
2	BBB	801	3HC	CCP-O6A-P2A-O4A
2	BBB	801	3HC	C5P-C6P-C7P-N8P
2	BBB	801	3HC	C6P-C5P-N4P-C3P
2	BBB	801	3HC	O5P-C5P-N4P-C3P
2	BBB	801	3HC	O1-C1-S1P-C2P
2	BBB	801	3HC	C2-C1-S1P-C2P
2	BBB	801	3HC	C1-C2-C3-O3
2	BBB	801	3HC	C1-C2-C3-C4
3	AAA	802	GOL	O1-C1-C2-C3
3	AAA	803	GOL	O1-C1-C2-C3
3	AAA	803	GOL	C1-C2-C3-O3
3	AAA	803	GOL	O2-C2-C3-O3
3	AAA	808	GOL	O1-C1-C2-O2
3	AAA	808	GOL	O1-C1-C2-C3
4	AAA	806	NAI	C5B-O5B-PA-O1A
4	AAA	806	NAI	O4B-C4B-C5B-O5B
4	AAA	806	NAI	C5D-O5D-PN-O2N
4	BBB	803	NAI	C5B-O5B-PA-O1A
2	AAA	801	3HC	O9P-C9P-N8P-C7P
2	AAA	801	3HC	O4B-C4B-C5B-O5B
3	AAA	804	GOL	C1-C2-C3-O3
3	AAA	805	GOL	O1-C1-C2-C3
3	AAA	805	GOL	C1-C2-C3-O3
3	BBB	802	GOL	O1-C1-C2-C3
3	AAA	802	GOL	O1-C1-C2-O2
3	AAA	803	GOL	O1-C1-C2-O2
3	AAA	804	GOL	O2-C2-C3-O3
4	AAA	806	NAI	C3B-C4B-C5B-O5B
4	BBB	803	NAI	O4B-C4B-C5B-O5B
2	AAA	801	3HC	O9P-C9P-CAP-OAP
2	AAA	801	3HC	C3B-C4B-C5B-O5B
2	AAA	801	3HC	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
3	AAA	805	GOL	O2-C2-C3-O3
2	AAA	801	3HC	O1-C1-S1P-C2P
4	AAA	806	NAI	C2D-C1D-N1N-C6N
2	BBB	801	3HC	P1A-O3A-P2A-O6A
2	AAA	801	3HC	C2-C1-S1P-C2P
4	AAA	806	NAI	C5B-O5B-PA-O3
4	AAA	806	NAI	C5D-O5D-PN-O3
2	BBB	801	3HC	P2A-O3A-P1A-O2A
4	AAA	806	NAI	O4D-C1D-N1N-C6N
3	AAA	805	GOL	O1-C1-C2-O2
4	AAA	806	NAI	C2D-C1D-N1N-C2N
4	BBB	803	NAI	O4D-C1D-N1N-C6N
3	BBB	802	GOL	O1-C1-C2-O2
2	BBB	801	3HC	S1P-C2P-C3P-N4P
4	BBB	803	NAI	C2D-C1D-N1N-C6N
2	AAA	801	3HC	C2P-C3P-N4P-C5P
4	AAA	806	NAI	O4D-C1D-N1N-C2N
2	AAA	801	3HC	C3P-C2P-S1P-C1
4	BBB	803	NAI	C3B-C4B-C5B-O5B
2	AAA	801	3HC	C3B-O3B-P3B-O8A
2	AAA	801	3HC	CCP-O6A-P2A-O3A
2	BBB	801	3HC	CCP-O6A-P2A-O3A
2	BBB	801	3HC	P2A-O3A-P1A-O1A
2	AAA	801	3HC	CBP-CCP-O6A-P2A

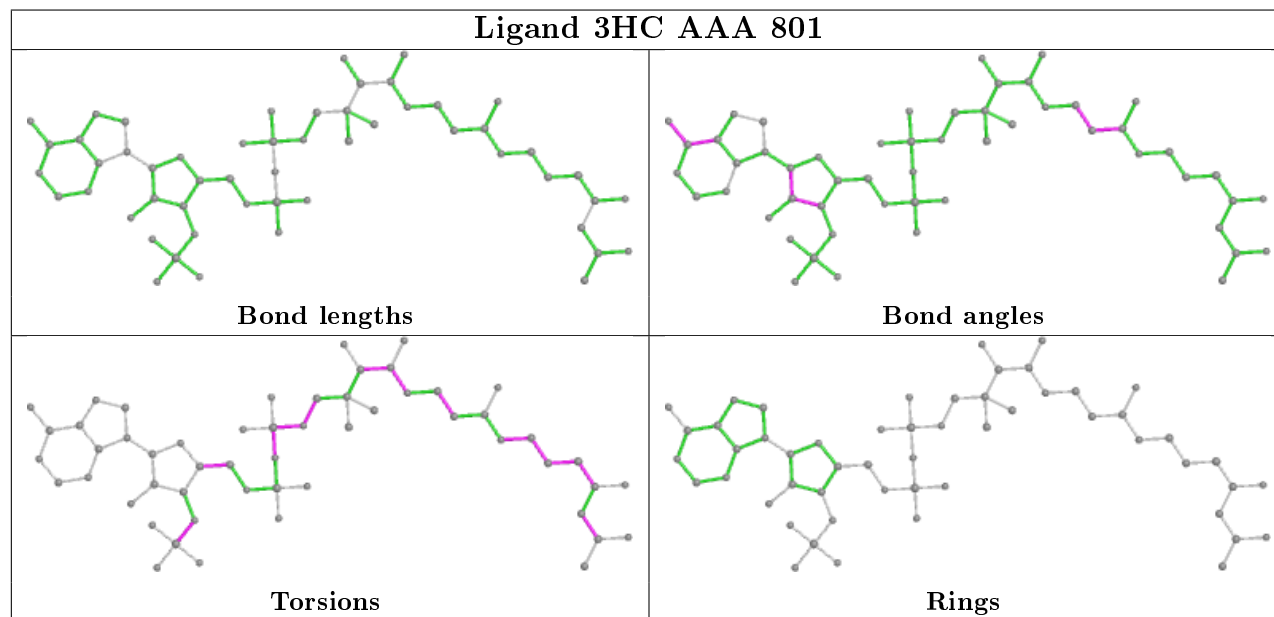
There are no ring outliers.

10 monomers are involved in 30 short contacts:

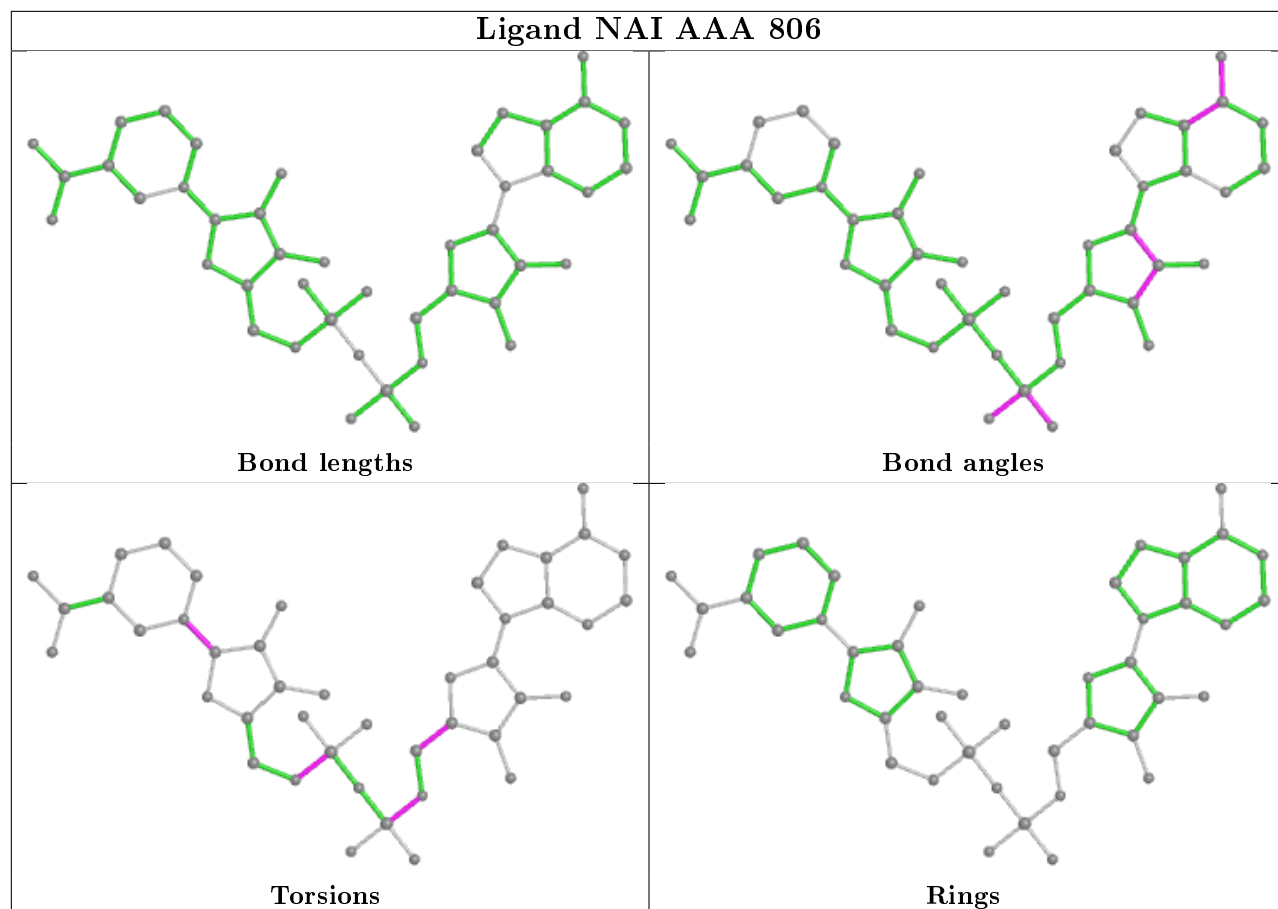
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	807	GOL	1	0
2	AAA	801	3HC	7	0
3	AAA	808	GOL	1	0
3	AAA	802	GOL	3	0
4	AAA	806	NAI	6	0
3	BBB	802	GOL	1	0
2	BBB	801	3HC	3	0
3	AAA	803	GOL	2	0
3	AAA	805	GOL	3	0
4	BBB	803	NAI	3	0

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

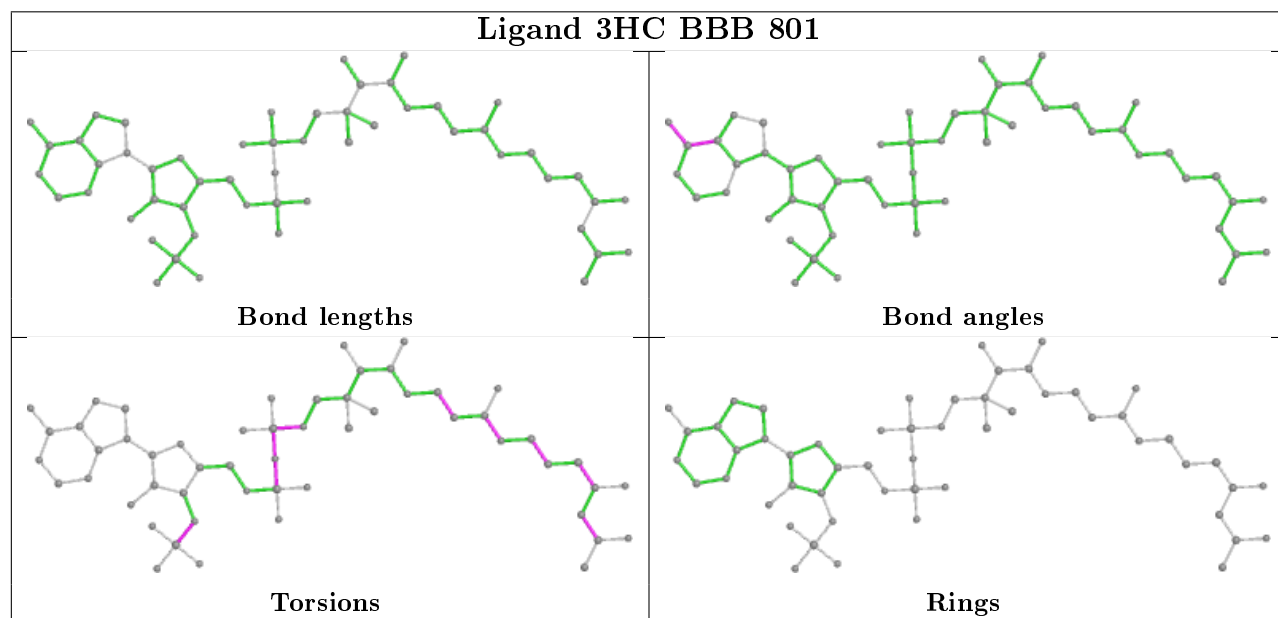
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

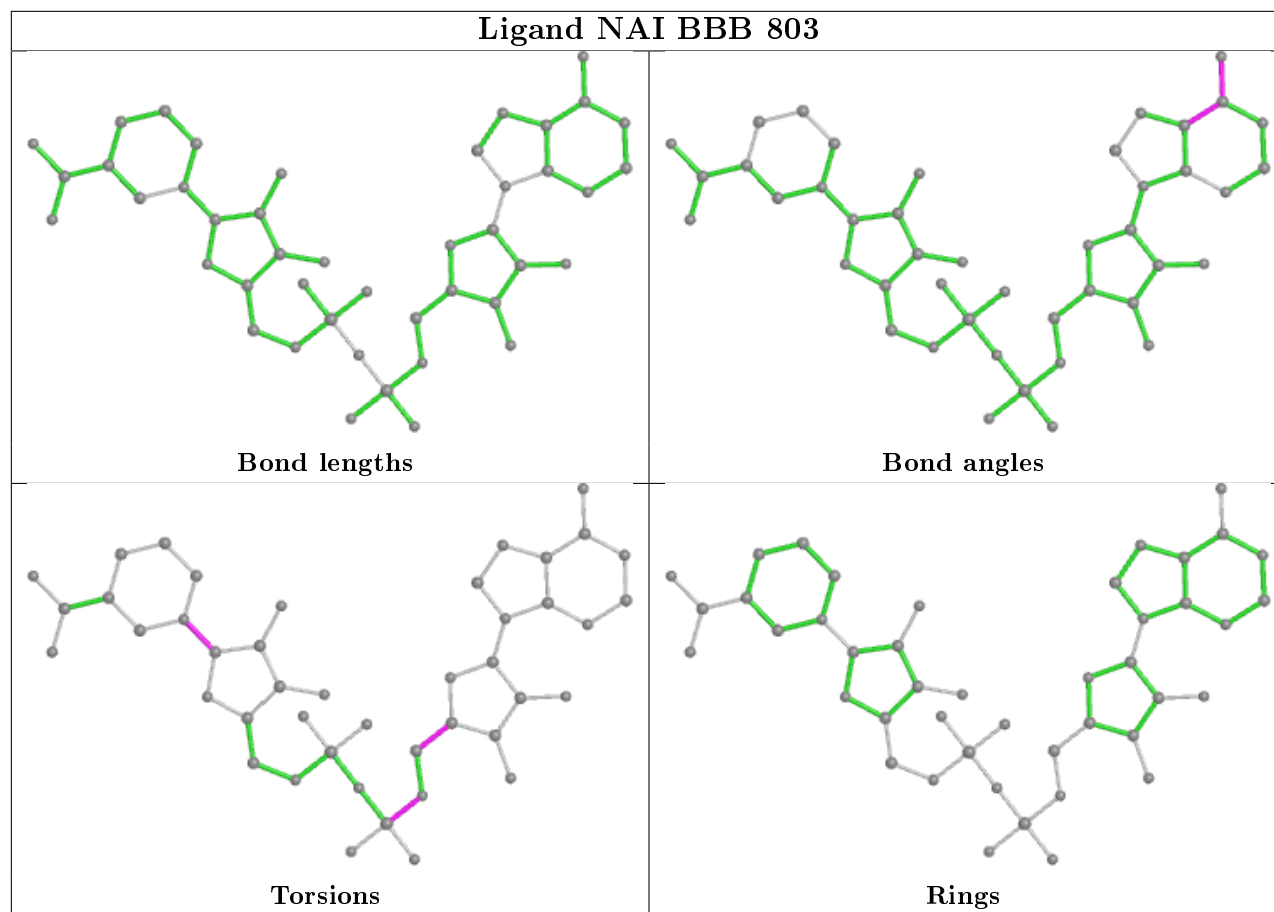


## Ligand NAI AAA 806



## Ligand 3HC BBB 801





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	723/742 (97%)	0.17	13 (1%) 68 66	21, 41, 94, 148	0
1	BBB	714/742 (96%)	0.20	28 (3%) 39 37	29, 60, 102, 143	0
All	All	1437/1484 (96%)	0.19	41 (2%) 51 49	21, 51, 99, 148	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	397	ALA	4.5
1	BBB	351	HIS	4.2
1	BBB	293	ALA	4.1
1	BBB	398	LEU	3.9
1	BBB	422	ASP	3.7
1	AAA	64	HIS	3.5
1	BBB	392	PHE	3.5
1	BBB	391	VAL	3.5
1	BBB	390	LYS	3.4
1	AAA	329	PRO	3.4
1	AAA	587	ARG	3.1
1	BBB	554	ASN	3.1
1	BBB	357	SER	3.1
1	BBB	402	GLY	3.1
1	AAA	327	SER	3.0
1	AAA	351	HIS	2.9
1	BBB	399	CYS	2.9
1	AAA	352	GLN	2.9
1	BBB	414	VAL	2.7
1	BBB	449	TYR	2.7
1	AAA	354	GLY	2.6
1	BBB	43	HIS	2.5
1	BBB	337	LYS	2.4
1	BBB	588	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	331	GLN	2.4
1	AAA	-3	ARG	2.4
1	BBB	395	LEU	2.4
1	BBB	385	MET	2.3
1	AAA	325	VAL	2.3
1	BBB	601	GLN	2.2
1	BBB	419	SER	2.2
1	AAA	328	ASP	2.2
1	BBB	377	VAL	2.1
1	BBB	450	SER	2.1
1	BBB	0	HIS	2.0
1	BBB	405	LEU	2.0
1	BBB	703	GLN	2.0
1	BBB	349	ARG	2.0
1	BBB	538	LEU	2.0
1	AAA	241	LYS	2.0
1	AAA	357	SER	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	AAA	808	6/6	0.69	0.27	68,75,81,86	0
3	GOL	AAA	807	6/6	0.71	0.21	62,72,77,80	0
2	3HC	AAA	801	54/54	0.72	0.30	43,119,156,160	0
3	GOL	AAA	803	6/6	0.76	0.22	70,76,79,80	0
3	GOL	AAA	805	6/6	0.82	0.21	79,83,83,86	0
3	GOL	BBB	802	6/6	0.83	0.20	64,79,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAI	AAA	806	44/44	0.85	0.20	42,54,69,80	0
2	3HC	BBB	801	54/54	0.87	0.17	50,72,82,85	0
5	SO4	BBB	804	5/5	0.87	0.22	77,86,91,94	0
3	GOL	AAA	804	6/6	0.88	0.20	49,55,57,59	0
3	GOL	AAA	802	6/6	0.90	0.30	54,65,66,67	0
4	NAI	BBB	803	44/44	0.94	0.18	45,58,63,66	0
5	SO4	AAA	809	5/5	0.97	0.11	47,48,49,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.