



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 12:33 PM EDT

PDB ID : 3B8G  
Title : Crysta structure of N-acetylglutamate synthase from Neisseria gonorrhoeae complexed with coenzyme A and N-acetyl-glutamate  
Authors : Shi, D.; Sagar, V.; Jin, Z.; Yu, X.; Caldovic, L.; Morizono, H.; Allewell, N.M.; Tuchman, M.  
Deposited on : 2007-11-01  
Resolution : 2.60 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

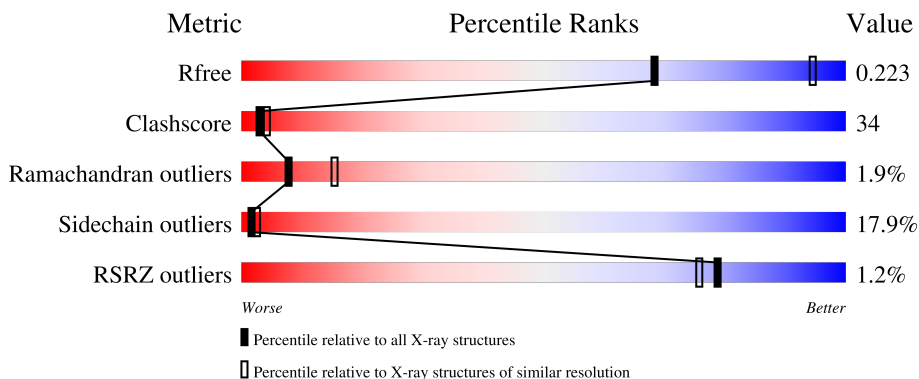
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	A	456	

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
2	COA	A	1	X	-	-	-
3	NLG	A	437	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3415 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.

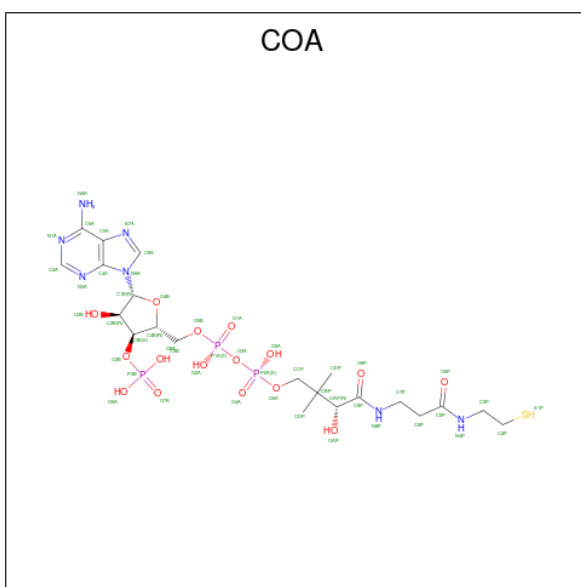
- Molecule 1 is a protein called Putative acetylglutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	3227	2012	595	611	9	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

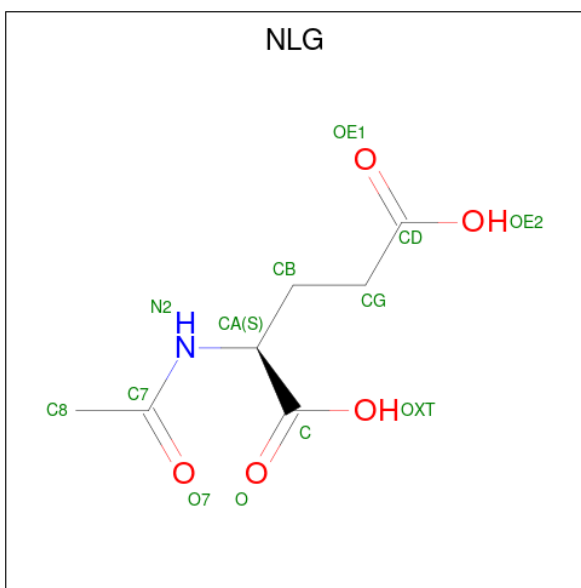
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q5FAK7
A	-18	GLY	-	expression tag	UNP Q5FAK7
A	-17	SER	-	expression tag	UNP Q5FAK7
A	-16	SER	-	expression tag	UNP Q5FAK7
A	-15	HIS	-	expression tag	UNP Q5FAK7
A	-14	HIS	-	expression tag	UNP Q5FAK7
A	-13	HIS	-	expression tag	UNP Q5FAK7
A	-12	HIS	-	expression tag	UNP Q5FAK7
A	-11	HIS	-	expression tag	UNP Q5FAK7
A	-10	HIS	-	expression tag	UNP Q5FAK7
A	-9	SER	-	expression tag	UNP Q5FAK7
A	-8	SER	-	expression tag	UNP Q5FAK7
A	-7	GLY	-	expression tag	UNP Q5FAK7
A	-6	LEU	-	expression tag	UNP Q5FAK7
A	-5	VAL	-	expression tag	UNP Q5FAK7
A	-4	PRO	-	expression tag	UNP Q5FAK7
A	-3	ARG	-	expression tag	UNP Q5FAK7
A	-2	GLY	-	expression tag	UNP Q5FAK7
A	-1	SER	-	expression tag	UNP Q5FAK7
A	0	HIS	-	expression tag	UNP Q5FAK7
A	312	ILE	VAL	engineered mutation	UNP Q5FAK7
A	336	ASN	ASP	engineered mutation	UNP Q5FAK7
A	427	SER	PRO	engineered mutation	UNP Q5FAK7

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	48	21	7	16	3	1	0	0

- Molecule 3 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula:  $C_7H_{11}NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	13	7	1	5	0	0

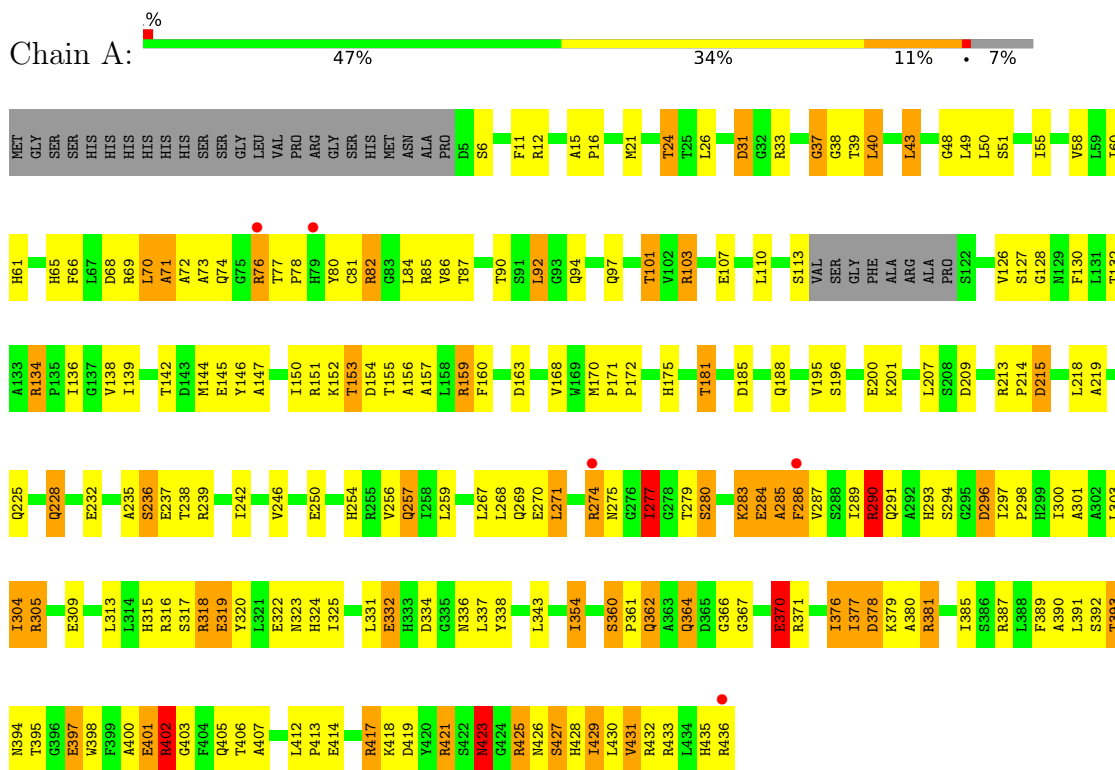
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total 127	O 127	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: Putative acetylglutamate synthase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.65Å 98.65Å 89.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.60) 99.3 (19.86-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.59Å)	Xtrriage
Refinement program	REFMAC 5.2.0005, CNS 1.2	Depositor
R, $R_{free}$	0.200 , 0.282 0.200 , 0.223	Depositor DCC
$R_{free}$ test set	760 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtrriage
Anisotropy	0.136	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: COA, NLG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.61	0/3280	1.21	21/4433 (0.5%)

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
1	A	0	5

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	A	290	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	A	43	LEU	CB-CG-CD2	-7.31	98.58	111.00
1	A	159	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	134	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	134	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	110	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	A	163	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	296	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	12	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	A	159	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	A	271	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	A	60	ILE	CB-CA-C	-5.68	100.24	111.60
1	A	31	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	A	402	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	92	LEU	CB-CG-CD1	-5.40	101.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	103	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	12	ARG	CG-CD-NE	-5.02	101.26	111.80
1	A	378	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	A	431	VAL	CB-CA-C	-5.01	101.89	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	ARG	Mainchain
1	A	283	LYS	Peptide
1	A	423	ASN	Mainchain
1	A	425	ARG	Mainchain
1	A	431	VAL	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3208	221	1
2	A	48	0	32	8	0
3	A	13	0	9	7	0
4	A	127	0	0	35	0
All	All	3415	0	3249	225	1

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 34.

All (225) 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:A:285:ALA:HB1	4:A:559:HOH:O	1.28	1.28
1:A:82:ARG:CB	1:A:82:ARG:HH11	1.54	1.19
1:A:82:ARG:NH1	1:A:82:ARG:HB2	1.56	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:OD1	1:A:188:GLN:HG2	1.50	1.12
1:A:259:LEU:HD21	1:A:270:GLU:HG2	1.35	1.09
1:A:213:ARG:HB3	1:A:214:PRO:HD2	1.38	1.06
1:A:213:ARG:CB	1:A:214:PRO:HD2	1.91	1.01
1:A:209:ASP:O	1:A:218:LEU:HD12	1.63	0.99
1:A:82:ARG:HH11	1:A:82:ARG:HB2	0.83	0.98
1:A:275:ASN:HB2	4:A:500:HOH:O	1.64	0.95
1:A:393:THR:HG23	1:A:394:ASN:ND2	1.81	0.95
1:A:287:VAL:HG21	1:A:371:ARG:HD3	1.49	0.94
1:A:403:GLY:O	1:A:432:ARG:HG3	1.66	0.94
1:A:24:THR:HG23	4:A:476:HOH:O	1.73	0.88
1:A:154:ASP:HA	4:A:535:HOH:O	1.74	0.86
1:A:320:TYR:HB3	4:A:517:HOH:O	1.76	0.85
1:A:175:HIS:CE1	1:A:181:THR:HG23	2.13	0.84
1:A:257:GLN:OE1	1:A:280:SER:HB2	1.78	0.82
1:A:31:ASP:OD2	1:A:33:ARG:HD3	1.80	0.81
2:A:1:COA:O5P	2:A:1:COA:H22	1.82	0.80
1:A:301:ALA:O	1:A:305:ARG:HG3	1.82	0.79
1:A:393:THR:CG2	1:A:394:ASN:ND2	2.46	0.79
1:A:284:GLU:HG2	1:A:284:GLU:O	1.82	0.78
1:A:318:ARG:HD3	4:A:493:HOH:O	1.83	0.78
1:A:103:ARG:HH21	1:A:127:SER:HB2	1.49	0.77
1:A:277:ILE:N	1:A:277:ILE:HD12	1.99	0.77
1:A:209:ASP:O	1:A:218:LEU:CD1	2.34	0.75
1:A:58:VAL:HG13	1:A:170:MET:HE3	1.69	0.75
1:A:128:GLY:HA3	1:A:130:PHE:CE1	2.22	0.74
1:A:370:GLU:OE2	1:A:402:ARG:HD3	1.87	0.74
1:A:254:HIS:HB3	4:A:447:HOH:O	1.87	0.74
1:A:136:ILE:HG21	1:A:139:ILE:HD11	1.70	0.74
1:A:425:ARG:NH1	3:A:437:NLG:CD	2.51	0.73
1:A:58:VAL:HG13	1:A:170:MET:CE	2.18	0.73
1:A:418:LYS:HZ3	1:A:421:ARG:HB2	1.54	0.73
1:A:82:ARG:HH11	1:A:82:ARG:CG	2.01	0.72
1:A:152:LYS:HE3	4:A:477:HOH:O	1.89	0.72
1:A:277:ILE:HD12	1:A:277:ILE:H	1.53	0.72
1:A:6:SER:HB2	4:A:544:HOH:O	1.92	0.70
1:A:213:ARG:CB	1:A:214:PRO:CD	2.70	0.69
1:A:300:ILE:O	1:A:304:ILE:HB	1.93	0.69
1:A:427:SER:OG	3:A:437:NLG:OE2	2.07	0.68
1:A:259:LEU:HD21	1:A:270:GLU:CG	2.21	0.67
1:A:275:ASN:CB	4:A:500:HOH:O	2.32	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:HB2	1:A:277:ILE:HD11	1.75	0.66
1:A:293:HIS:HB3	4:A:485:HOH:O	1.95	0.66
1:A:71:ALA:O	1:A:72:ALA:C	2.33	0.66
1:A:316:ARG:O	1:A:317:SER:HB3	1.94	0.66
1:A:286:PHE:O	1:A:286:PHE:CD1	2.49	0.66
1:A:58:VAL:CG1	1:A:170:MET:CE	2.74	0.65
1:A:66:PHE:HD1	1:A:69:ARG:NH2	1.93	0.65
1:A:218:LEU:HD23	1:A:218:LEU:C	2.16	0.65
1:A:159:ARG:HB2	1:A:159:ARG:NH1	2.12	0.64
1:A:159:ARG:HB2	1:A:159:ARG:HH11	1.63	0.64
1:A:315:HIS:CD2	1:A:316:ARG:O	2.50	0.64
1:A:159:ARG:HH11	1:A:159:ARG:CB	2.11	0.64
1:A:58:VAL:CG1	1:A:170:MET:HE3	2.28	0.63
1:A:38:GLY:HA2	4:A:518:HOH:O	1.99	0.62
1:A:175:HIS:ND1	1:A:181:THR:HG23	2.13	0.62
1:A:429:ILE:HD12	1:A:430:LEU:N	2.14	0.62
1:A:40:LEU:O	1:A:40:LEU:HD22	1.99	0.61
1:A:24:THR:CG2	4:A:476:HOH:O	2.42	0.61
1:A:387:ARG:CD	4:A:495:HOH:O	2.47	0.61
1:A:101:THR:HG21	4:A:508:HOH:O	2.00	0.60
1:A:21:MET:HE2	1:A:55:ILE:HD13	1.81	0.60
1:A:84:LEU:O	1:A:144:MET:HE2	2.02	0.60
1:A:228:GLN:HA	1:A:228:GLN:NE2	2.16	0.60
1:A:397:GLU:OE2	2:A:1:COA:N1A	2.35	0.59
1:A:433:ARG:HG2	4:A:527:HOH:O	2.02	0.59
2:A:1:COA:O9P	2:A:1:COA:H62	2.01	0.59
2:A:1:COA:O9A	4:A:515:HOH:O	2.17	0.59
1:A:66:PHE:CD1	1:A:69:ARG:NH2	2.71	0.59
1:A:103:ARG:NH1	1:A:107:GLU:OE1	2.36	0.59
1:A:418:LYS:NZ	1:A:421:ARG:HB2	2.17	0.58
1:A:425:ARG:NH1	3:A:437:NLG:OE2	2.37	0.58
1:A:289:ILE:HD11	1:A:331:LEU:HD12	1.85	0.58
1:A:84:LEU:O	1:A:144:MET:CE	2.52	0.58
1:A:257:GLN:NE2	4:A:545:HOH:O	2.33	0.57
1:A:68:ASP:OD2	1:A:80:TYR:OH	2.22	0.57
1:A:185:ASP:OD1	1:A:188:GLN:CG	2.41	0.57
1:A:242:ILE:O	1:A:246:VAL:HG23	2.03	0.56
1:A:103:ARG:NH2	1:A:127:SER:HB2	2.19	0.56
1:A:246:VAL:O	1:A:250:GLU:HG3	2.05	0.56
1:A:61:HIS:CE1	1:A:172:PRO:HD3	2.41	0.56
1:A:284:GLU:O	1:A:284:GLU:CG	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD13	1:A:94:GLN:OE1	2.04	0.56
1:A:419:ASP:HB3	4:A:471:HOH:O	2.05	0.55
1:A:136:ILE:CG2	1:A:139:ILE:HD11	2.36	0.55
1:A:397:GLU:OE2	2:A:1:COA:C2A	2.55	0.55
1:A:81:CYS:O	1:A:82:ARG:HB3	2.07	0.55
1:A:150:ILE:HG21	1:A:153:THR:HG22	1.88	0.55
1:A:286:PHE:O	1:A:287:VAL:HG13	2.06	0.55
1:A:389:PHE:HD1	1:A:429:ILE:HD13	1.71	0.55
1:A:128:GLY:HA3	1:A:130:PHE:CZ	2.42	0.55
1:A:297:ILE:CD1	4:A:478:HOH:O	2.54	0.55
1:A:286:PHE:O	1:A:286:PHE:HD1	1.89	0.55
1:A:387:ARG:HD3	4:A:495:HOH:O	2.06	0.54
1:A:58:VAL:CG1	1:A:170:MET:HE1	2.37	0.54
1:A:82:ARG:CB	1:A:82:ARG:NH1	2.38	0.53
1:A:393:THR:HG23	1:A:394:ASN:CG	2.28	0.53
1:A:144:MET:HB3	1:A:147:ALA:HB3	1.90	0.53
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.73	0.53
1:A:287:VAL:HG21	1:A:371:ARG:CD	2.31	0.53
1:A:354:ILE:CG2	1:A:390:ALA:HB2	2.39	0.52
1:A:92:LEU:C	1:A:92:LEU:HD13	2.30	0.52
1:A:389:PHE:HD1	1:A:429:ILE:CD1	2.23	0.52
1:A:407:ALA:HB3	1:A:429:ILE:HG13	1.92	0.52
1:A:33:ARG:CZ	1:A:207:LEU:HD22	2.40	0.52
1:A:38:GLY:CA	4:A:518:HOH:O	2.58	0.51
1:A:68:ASP:OD1	1:A:68:ASP:N	2.42	0.51
1:A:200:GLU:HA	1:A:254:HIS:CD2	2.45	0.51
1:A:297:ILE:N	1:A:298:PRO:HD2	2.25	0.51
1:A:315:HIS:HD2	1:A:316:ARG:O	1.89	0.51
1:A:21:MET:SD	1:A:271:LEU:HD22	2.51	0.51
1:A:366:GLY:N	4:A:484:HOH:O	2.35	0.51
1:A:290:ARG:NH1	1:A:332:GLU:OE1	2.44	0.51
1:A:354:ILE:HB	1:A:376:ILE:HD11	1.93	0.51
1:A:87:THR:O	1:A:146:TYR:HB2	2.11	0.50
1:A:387:ARG:HD2	4:A:495:HOH:O	2.09	0.50
1:A:391:LEU:HD12	1:A:391:LEU:N	2.26	0.50
1:A:250:GLU:OE2	1:A:283:LYS:NZ	2.30	0.49
1:A:397:GLU:OE2	2:A:1:COA:H2A	2.09	0.49
1:A:71:ALA:O	1:A:73:ALA:N	2.45	0.49
1:A:325:ILE:O	1:A:325:ILE:HG13	2.13	0.49
1:A:360:SER:HB2	1:A:362:GLN:HG3	1.94	0.49
1:A:423:ASN:HB3	1:A:425:ARG:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLN:O	1:A:101:THR:HG22	2.13	0.49
1:A:134:ARG:HG3	1:A:134:ARG:NH1	2.28	0.49
1:A:294:SER:HA	4:A:478:HOH:O	2.12	0.48
2:A:1:COA:H8A	4:A:459:HOH:O	2.11	0.48
1:A:40:LEU:HB2	4:A:529:HOH:O	2.13	0.48
1:A:393:THR:HG23	1:A:394:ASN:HD21	1.72	0.48
1:A:213:ARG:HB3	1:A:214:PRO:CD	2.27	0.48
1:A:76:ARG:HH22	1:A:90:THR:HG22	1.79	0.48
1:A:354:ILE:CD1	1:A:376:ILE:HG12	2.44	0.48
1:A:425:ARG:HH12	3:A:437:NLG:CD	2.27	0.47
1:A:425:ARG:HH12	3:A:437:NLG:HGC2	1.78	0.47
1:A:155:THR:HG22	1:A:159:ARG:NH2	2.29	0.47
1:A:15:ALA:N	1:A:16:PRO:HD2	2.28	0.47
1:A:37:GLY:N	4:A:529:HOH:O	2.47	0.47
1:A:58:VAL:HG11	1:A:170:MET:HE1	1.95	0.47
1:A:426:ASN:O	1:A:427:SER:C	2.50	0.47
1:A:33:ARG:HD2	1:A:65:HIS:CG	2.50	0.47
1:A:213:ARG:O	1:A:215:ASP:N	2.48	0.47
1:A:315:HIS:CD2	1:A:315:HIS:C	2.88	0.47
1:A:218:LEU:HD23	1:A:219:ALA:C	2.36	0.47
1:A:412:LEU:O	1:A:413:PRO:C	2.50	0.47
1:A:82:ARG:NH1	1:A:82:ARG:CG	2.69	0.46
1:A:336:ASN:HB2	1:A:338:TYR:CE1	2.51	0.46
1:A:343:LEU:HD21	1:A:380:ALA:HA	1.97	0.46
1:A:138:VAL:HG13	1:A:142:THR:C	2.36	0.46
1:A:200:GLU:HB2	4:A:476:HOH:O	2.15	0.46
1:A:296:ASP:O	1:A:300:ILE:HG13	2.16	0.46
1:A:21:MET:HE2	1:A:55:ILE:CD1	2.46	0.46
1:A:397:GLU:CD	1:A:397:GLU:H	2.18	0.46
1:A:200:GLU:O	1:A:254:HIS:HB2	2.16	0.46
1:A:225:GLN:HA	4:A:513:HOH:O	2.16	0.46
1:A:80:TYR:CZ	1:A:85:ARG:HD2	2.50	0.45
1:A:303:LEU:HD12	1:A:303:LEU:O	2.16	0.45
1:A:318:ARG:O	1:A:322:GLU:HB2	2.17	0.45
1:A:425:ARG:HH12	3:A:437:NLG:CG	2.29	0.45
1:A:270:GLU:HB2	1:A:277:ILE:CD1	2.44	0.45
1:A:323:ASN:C	1:A:324:HIS:HD2	2.20	0.45
1:A:397:GLU:O	1:A:398:TRP:C	2.54	0.45
1:A:38:GLY:C	4:A:518:HOH:O	2.54	0.45
1:A:134:ARG:HD3	1:A:151:ARG:HB2	1.99	0.45
1:A:297:ILE:HD11	4:A:478:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ALA:HB3	1:A:429:ILE:CG1	2.47	0.45
1:A:380:ALA:O	1:A:385:ILE:HB	2.17	0.45
1:A:70:LEU:HD13	1:A:94:GLN:CD	2.36	0.44
1:A:389:PHE:CD1	1:A:429:ILE:CD1	3.00	0.44
1:A:397:GLU:HA	1:A:400:ALA:HB3	2.00	0.44
1:A:316:ARG:HA	1:A:320:TYR:HD1	1.82	0.44
1:A:418:LYS:NZ	1:A:421:ARG:CB	2.80	0.44
1:A:77:THR:HA	1:A:78:PRO:HD2	1.86	0.44
1:A:414:GLU:O	1:A:417:ARG:HB3	2.17	0.44
1:A:33:ARG:NH1	1:A:207:LEU:HD13	2.33	0.44
1:A:367:GLY:HA2	2:A:1:COA:O1A	2.18	0.44
1:A:377:ILE:HG12	1:A:378:ASP:N	2.33	0.43
1:A:219:ALA:O	1:A:279:THR:HG23	2.18	0.43
1:A:304:ILE:HD12	1:A:304:ILE:HA	1.43	0.43
1:A:320:TYR:CB	4:A:517:HOH:O	2.51	0.43
1:A:136:ILE:HD12	1:A:147:ALA:HB1	1.99	0.43
1:A:33:ARG:HD2	1:A:65:HIS:CB	2.48	0.43
1:A:21:MET:HE2	1:A:21:MET:HB3	1.80	0.43
1:A:26:LEU:HD12	1:A:201:LYS:HD2	2.00	0.43
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.83	0.43
1:A:286:PHE:O	1:A:287:VAL:CG1	2.66	0.43
1:A:324:HIS:CD2	1:A:324:HIS:N	2.85	0.43
1:A:332:GLU:HA	1:A:336:ASN:O	2.19	0.43
1:A:304:ILE:HD12	1:A:313:LEU:HD12	2.01	0.42
1:A:213:ARG:HB2	1:A:214:PRO:HD2	1.90	0.42
1:A:354:ILE:HD12	1:A:376:ILE:HG12	2.01	0.42
1:A:139:ILE:HD12	1:A:144:MET:CG	2.50	0.42
1:A:168:VAL:HG11	1:A:170:MET:HE2	2.01	0.42
1:A:213:ARG:HG2	1:A:219:ALA:HB2	2.01	0.42
1:A:397:GLU:O	1:A:401:GLU:HB2	2.19	0.42
1:A:236:SER:O	1:A:239:ARG:HB3	2.19	0.42
1:A:50:LEU:O	1:A:51:SER:C	2.55	0.42
1:A:86:VAL:HG13	1:A:145:GLU:HG3	2.02	0.42
1:A:235:ALA:O	1:A:236:SER:C	2.57	0.42
1:A:195:VAL:O	1:A:196:SER:C	2.58	0.42
1:A:218:LEU:HD23	1:A:219:ALA:N	2.35	0.42
1:A:392:SER:O	1:A:428:HIS:N	2.49	0.42
1:A:31:ASP:OD1	1:A:33:ARG:NH1	2.52	0.41
1:A:343:LEU:HD23	1:A:379:LYS:HG2	2.02	0.41
1:A:285:ALA:CB	4:A:559:HOH:O	2.13	0.41
1:A:319:GLU:O	1:A:320:TYR:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASN:C	1:A:324:HIS:CD2	2.93	0.41
1:A:175:HIS:CE1	1:A:181:THR:CG2	2.93	0.41
1:A:201:LYS:HB2	1:A:201:LYS:HE2	1.62	0.41
1:A:354:ILE:HG22	1:A:389:PHE:O	2.20	0.41
1:A:269:GLN:HG2	1:A:277:ILE:HG13	2.03	0.41
1:A:425:ARG:HH11	3:A:437:NLG:CD	2.30	0.41
1:A:15:ALA:HB3	1:A:16:PRO:CD	2.50	0.41
1:A:157:ALA:O	1:A:160:PHE:HB3	2.21	0.41
1:A:361:PRO:HA	1:A:364:GLN:OE1	2.21	0.41
1:A:48:GLY:O	1:A:51:SER:HB3	2.21	0.41
1:A:68:ASP:HA	1:A:71:ALA:HB3	2.03	0.41
1:A:418:LYS:HZ3	1:A:421:ARG:CB	2.28	0.40
1:A:325:ILE:HD12	1:A:325:ILE:HA	1.93	0.40
1:A:132:THR:HA	1:A:175:HIS:O	2.21	0.40
1:A:150:ILE:CG2	1:A:153:THR:HG22	2.52	0.40
1:A:156:ALA:N	4:A:444:HOH:O	2.11	0.40
1:A:218:LEU:C	1:A:218:LEU:CD2	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:NH1	1:A:305:ARG:NH1[5_655]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	420/456 (92%)	381 (91%)	31 (7%)	8 (2%)	<b>8</b> <b>15</b>

All (8) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	284	GLU
1	A	427	SER
1	A	236	SER
1	A	285	ALA
1	A	71	ALA
1	A	277	ILE
1	A	370	GLU
1	A	37	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	A	330/355 (93%)	271 (82%)	59 (18%)	<b>2</b> <b>2</b>

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	24	THR
1	A	39	THR
1	A	40	LEU
1	A	43	LEU
1	A	49	LEU
1	A	70	LEU
1	A	74	GLN
1	A	76	ARG
1	A	82	ARG
1	A	101	THR
1	A	113	SER
1	A	126	VAL
1	A	153	THR
1	A	171	PRO
1	A	181	THR
1	A	215	ASP
1	A	228	GLN
1	A	232	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	237	GLU
1	A	238	THR
1	A	256	VAL
1	A	257	GLN
1	A	267	LEU
1	A	268	LEU
1	A	274	ARG
1	A	277	ILE
1	A	280	SER
1	A	286	PHE
1	A	290	ARG
1	A	291	GLN
1	A	304	ILE
1	A	305	ARG
1	A	309	GLU
1	A	318	ARG
1	A	319	GLU
1	A	332	GLU
1	A	334	ASP
1	A	337	LEU
1	A	354	ILE
1	A	360	SER
1	A	362	GLN
1	A	364	GLN
1	A	370	GLU
1	A	376	ILE
1	A	377	ILE
1	A	381	ARG
1	A	393	THR
1	A	395	THR
1	A	397	GLU
1	A	401	GLU
1	A	402	ARG
1	A	405	GLN
1	A	406	THR
1	A	421	ARG
1	A	423	ASN
1	A	429	ILE
1	A	435	HIS
1	A	436	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	161	GLN
1	A	166	ASN
1	A	228	GLN
1	A	275	ASN
1	A	315	HIS
1	A	362	GLN
1	A	394	ASN
1	A	423	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	NLG	A	437	-	12,12,12	1.01	0	15,15,15	2.16	5 (33%)
2	COA	A	1	-	41,50,50	1.61	5 (12%)	52,75,75	1.76	17 (32%)

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	NLG	A	437	-	-	0/13/13/13	-
2	COA	A	1	-	1/1/11/13	16/44/64/64	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	COA	C3P-N4P	-5.57	1.33	1.46
2	A	1	COA	P3B-O7A	4.78	1.66	1.50
2	A	1	COA	O4B-C1B	3.34	1.45	1.41
2	A	1	COA	P3B-O3B	2.46	1.64	1.59
2	A	1	COA	P3B-O8A	2.44	1.64	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	437	NLG	CB-CA-N2	-5.00	100.77	110.88
3	A	437	NLG	CB-CA-C	-4.53	99.44	110.35
2	A	1	COA	C6P-C5P-N4P	-4.04	109.63	116.42
2	A	1	COA	N6A-C6A-N1A	3.53	125.90	118.57
2	A	1	COA	C2P-C3P-N4P	3.29	119.82	112.31
2	A	1	COA	N3A-C2A-N1A	-2.92	124.12	128.68
2	A	1	COA	CAP-C9P-N8P	-2.87	110.87	116.58
2	A	1	COA	C7P-N8P-C9P	-2.74	117.70	122.59
2	A	1	COA	C1B-N9A-C4A	-2.69	121.92	126.64
2	A	1	COA	C5A-C6A-N6A	-2.58	116.43	120.35
2	A	1	COA	O9A-P3B-O8A	2.55	117.37	107.64
3	A	437	NLG	CG-CB-CA	2.55	117.91	113.16
2	A	1	COA	CEP-CBP-CDP	2.44	114.14	109.17
3	A	437	NLG	OE2-CD-OE1	-2.35	117.44	123.30
2	A	1	COA	O8A-P3B-O7A	-2.32	101.60	110.68
2	A	1	COA	O3B-C3B-C2B	-2.25	103.54	111.68
2	A	1	COA	CEP-CBP-CCP	-2.22	104.61	108.23
2	A	1	COA	C5B-C4B-C3B	2.16	121.56	114.40
2	A	1	COA	O4B-C4B-C5B	-2.14	102.33	109.37
3	A	437	NLG	O7-C7-C8	-2.13	118.11	122.06
2	A	1	COA	P2A-O3A-P1A	-2.07	125.71	132.83
2	A	1	COA	CEP-CBP-CAP	-2.02	105.33	108.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1	COA	CAP

All (16) torsion outliers are listed below:

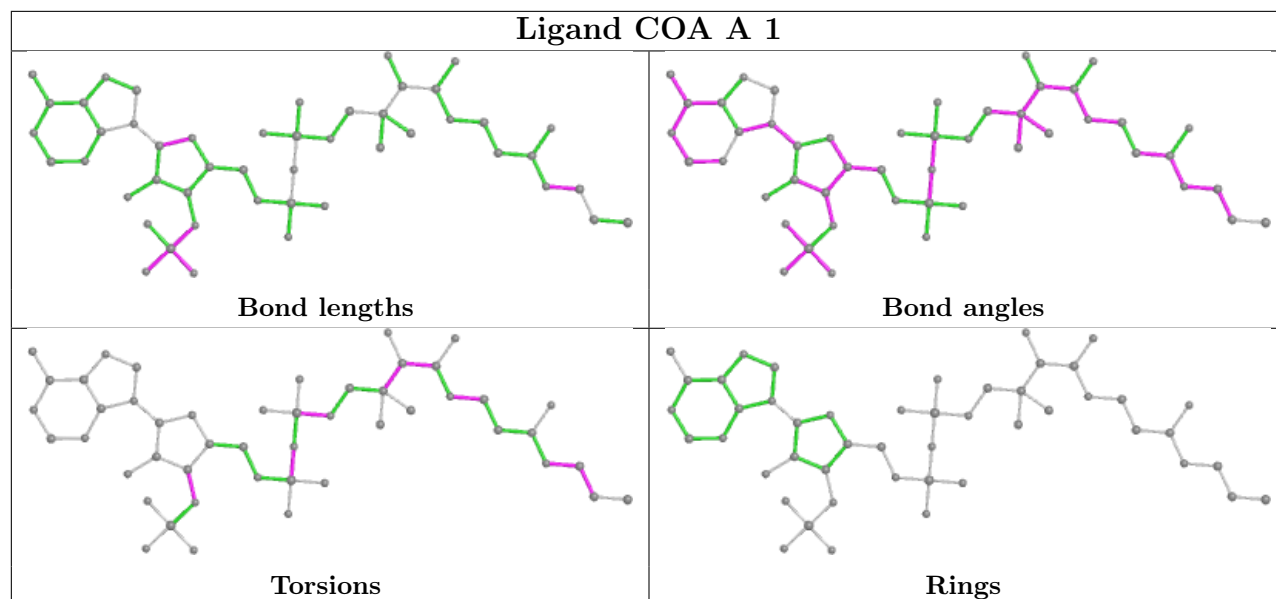
Mol	Chain	Res	Type	Atoms
2	A	1	COA	CCP-O6A-P2A-O4A
2	A	1	COA	OAP-CAP-CBP-CCP
2	A	1	COA	C9P-CAP-CBP-CCP
2	A	1	COA	OAP-CAP-CBP-CDP
2	A	1	COA	C9P-CAP-CBP-CDP
2	A	1	COA	C9P-CAP-CBP-CEP
2	A	1	COA	C2P-C3P-N4P-C5P
2	A	1	COA	S1P-C2P-C3P-N4P
2	A	1	COA	C6P-C7P-N8P-C9P
2	A	1	COA	C2B-C3B-O3B-P3B
2	A	1	COA	OAP-CAP-CBP-CEP
2	A	1	COA	C4B-C3B-O3B-P3B
2	A	1	COA	CCP-O6A-P2A-O3A
2	A	1	COA	P2A-O3A-P1A-O2A
2	A	1	COA	P2A-O3A-P1A-O1A
2	A	1	COA	O9P-C9P-CAP-OAP

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	437	NLG	7	0
2	A	1	COA	8	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.



## 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, 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	A	424/456 (92%)	-0.53	5 (1%) 79 76	16, 32, 54, 73	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436	ARG	3.9
1	A	286	PHE	3.0
1	A	274	ARG	2.5
1	A	76	ARG	2.3
1	A	79	HIS	2.2

### 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](#)

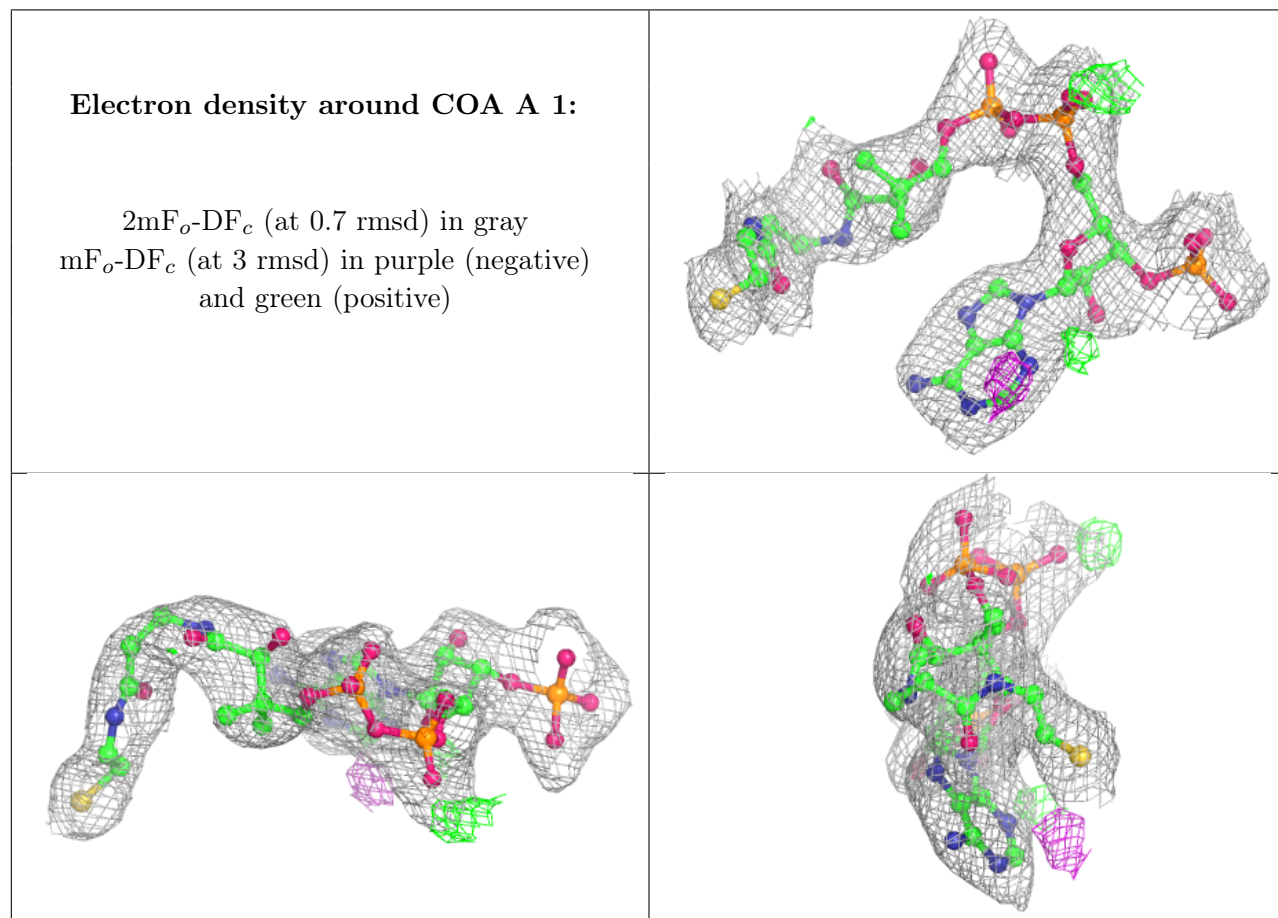
There are no monosaccharides in this entry.

### 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	NLG	A	437	13/13	0.95	0.13	38,44,49,50	0
2	COA	A	1	48/48	0.96	0.10	29,48,57,66	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.