



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:20 AM UTC

PDB ID : 3D2P / pdb_00003d2p
Title : Crystal structure of N-acetylglutamate synthase from *Neisseria gonorrhoeae* complexed with coenzyme A and L-arginine
Authors : Shi, D.; Min, L.; Jin, Z.; Allewell, N.M.; Tuchman, M.
Deposited on : 2008-05-08
Resolution : 2.56 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

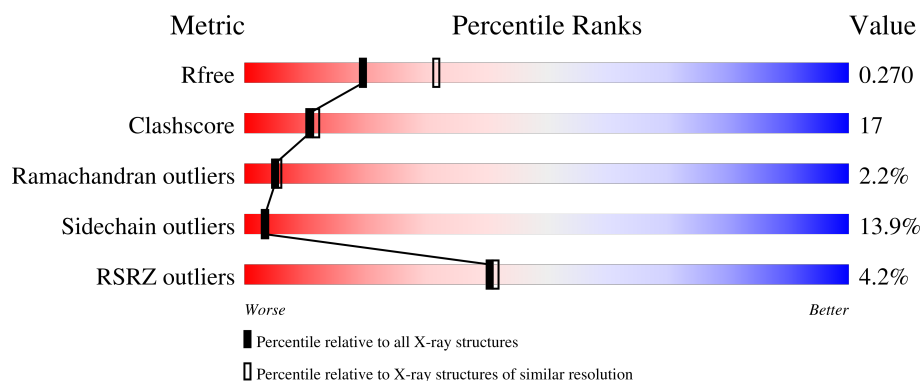
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

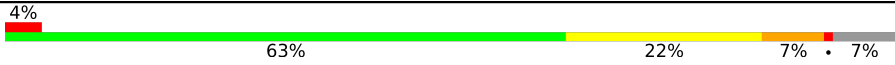
The reported resolution of this entry is 2.56 Å.

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}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	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	437	X	-	-	-
2	COA	B	437	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6745 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
1	A	424	Total	C	N	O	S	0	0	0
			3223	2016	593	605	9			
1	B	424	Total	C	N	O	S	0	0	0
			3223	2016	593	605	9			

There are 46 discrepancies between the modelled and reference sequences:

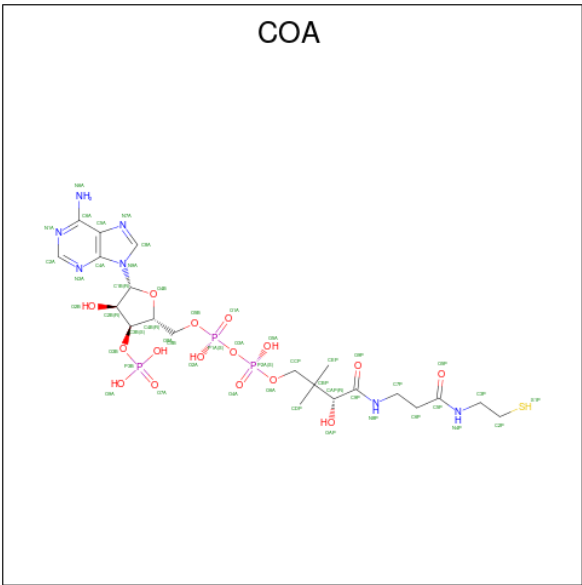
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q5FAK7
A	-18	GLY	-	expression tag	UNP Q5FAK7
A	-17	SER	-	expression tag	UNP Q5FAK7
A	-16	SER	-	expression tag	UNP Q5FAK7
A	-15	HIS	-	expression tag	UNP Q5FAK7
A	-14	HIS	-	expression tag	UNP Q5FAK7
A	-13	HIS	-	expression tag	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
B	-19	MET	-	expression tag	UNP Q5FAK7
B	-18	GLY	-	expression tag	UNP Q5FAK7

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

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



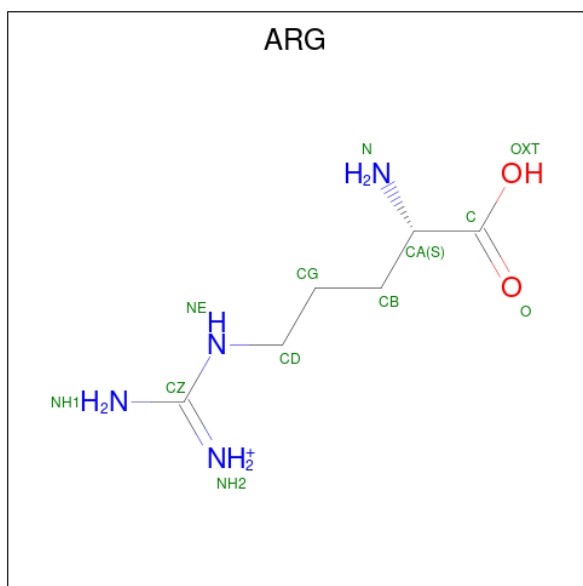
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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

- Molecule 3 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	4	2		
3	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	105	Total	O	0	0
			105	105		

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants a, b, c, α , β , γ	107.05Å 107.05Å 185.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.56 20.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-2.56) 90.6 (20.00-2.56)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.273 0.212 , 0.270	Depositor DCC
R_{free} test set	1786 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6745	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	1.05	5/3277 (0.2%)	1.17	15/4430 (0.3%)
1	B	1.02	3/3277 (0.1%)	1.18	13/4430 (0.3%)
All	All	1.04	8/6554 (0.1%)	1.18	28/8860 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	ARG	NE-CZ	19.47	1.54	1.33
1	A	387	ARG	CZ-NH1	14.97	1.53	1.32
1	A	350	ASP	C-N	13.63	1.52	1.33
1	B	429	ILE	CA-CB	8.64	1.64	1.53
1	B	171	PRO	CA-C	5.48	1.57	1.52
1	A	433	ARG	CZ-NH1	5.48	1.40	1.32
1	A	62	GLY	N-CA	5.36	1.50	1.44
1	B	287	VAL	N-CA	5.28	1.52	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	ARG	NE-CZ-NH1	-11.65	109.84	121.50
1	B	277	ILE	N-CA-C	-10.87	95.56	108.82
1	A	320	TYR	N-CA-C	-10.01	101.40	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ILE	N-CA-C	-8.40	97.03	108.96
1	B	286	PHE	N-CA-C	-7.61	100.48	110.53
1	B	319	GLU	N-CA-C	7.44	120.38	109.07
1	A	350	ASP	CA-C-O	7.07	129.10	120.55
1	A	387	ARG	CD-NE-CZ	-6.59	115.17	124.40
1	A	38	GLY	N-CA-C	-6.39	107.64	114.67
1	A	388	LEU	N-CA-C	6.21	118.83	108.96
1	A	286	PHE	N-CA-C	-6.02	102.17	110.35
1	B	320	TYR	N-CA-C	-5.65	106.23	113.23
1	B	186	MET	N-CA-C	5.64	117.11	111.07
1	B	287	VAL	CB-CA-C	-5.55	102.19	111.29
1	A	131	LEU	CA-C-N	-5.37	115.59	123.00
1	A	131	LEU	C-N-CA	-5.37	115.59	123.00
1	B	134	ARG	CA-C-N	5.31	125.07	119.76
1	B	134	ARG	C-N-CA	5.31	125.07	119.76
1	B	386	SER	N-CA-C	-5.30	107.47	114.31
1	A	392	SER	N-CA-C	5.28	117.98	108.48
1	B	315	HIS	N-CA-C	5.21	117.53	111.02
1	B	109	ALA	N-CA-C	-5.21	105.69	111.36
1	A	433	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	A	77	THR	CA-C-N	5.10	125.02	119.76
1	A	77	THR	C-N-CA	5.10	125.02	119.76
1	A	170	MET	N-CA-C	5.10	117.56	109.40
1	B	429	ILE	CB-CA-C	5.08	118.42	111.31
1	B	431	VAL	CB-CA-C	-5.01	102.94	110.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	ARG	Sidechain

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	3223	0	3213	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3223	0	3213	105	0
2	A	48	0	32	9	0
2	B	48	0	32	8	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
4	A	74	0	0	6	0
4	B	105	0	0	15	0
All	All	6745	0	6514	219	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 17.

All (219) 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:407:ALA:HB1	1:A:411:GLU:OE2	1.27	1.26
1:B:84:LEU:HB2	4:B:482:HOH:O	1.38	1.22
1:A:119:ARG:HG2	1:A:119:ARG:HH11	1.10	1.09
1:B:119:ARG:HG2	1:B:119:ARG:HH11	0.97	1.09
1:A:68:ASP:OD1	1:A:85:ARG:NH1	1.88	1.04
1:A:219:ALA:O	1:A:220:GLU:HB3	1.59	1.02
1:B:21:MET:O	1:B:24:THR:HB	1.63	0.99
1:B:119:ARG:HG2	1:B:119:ARG:NH1	1.73	0.95
1:A:119:ARG:HG2	1:A:119:ARG:NH1	1.76	0.93
1:A:101:THR:HB	4:B:513:HOH:O	1.68	0.93
1:B:316:ARG:HG2	1:B:317:SER:H	1.36	0.91
1:B:219:ALA:O	1:B:220:GLU:HB2	1.72	0.89
1:A:407:ALA:CB	1:A:411:GLU:OE2	2.20	0.89
2:A:437:COA:HN8	2:A:437:COA:H131	1.39	0.88
1:B:68:ASP:OD1	1:B:85:ARG:NH1	2.07	0.87
1:B:354:ILE:HD12	1:B:376:ILE:HG12	1.59	0.85
1:A:259:LEU:HD21	1:A:270:GLU:HG2	1.61	0.83
1:A:318:ARG:O	1:A:319:GLU:OE1	1.97	0.82
1:B:316:ARG:HG2	1:B:317:SER:N	1.93	0.82
1:A:314:LEU:HD13	1:A:315:HIS:H	1.45	0.81
1:A:119:ARG:HH11	1:A:119:ARG:CG	1.92	0.81
2:B:437:COA:HN8	2:B:437:COA:H131	1.45	0.81
1:B:219:ALA:O	1:B:220:GLU:CB	2.29	0.79
1:A:407:ALA:HB2	4:A:439:HOH:O	1.80	0.79
1:B:307:LEU:HD21	2:B:437:COA:H61	1.65	0.78
1:B:407:ALA:HB2	1:B:431:VAL:HG23	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:HG3	1:A:12:ARG:HH11	1.49	0.78
1:B:84:LEU:HD13	4:B:482:HOH:O	1.86	0.76
1:A:341:ALA:HB1	1:A:354:ILE:HD11	1.68	0.75
1:A:412:LEU:HD21	1:A:429:ILE:HD13	1.67	0.75
1:B:318:ARG:O	1:B:319:GLU:CD	2.30	0.75
1:B:254:HIS:HB3	4:B:464:HOH:O	1.87	0.75
1:B:380:ALA:O	1:B:384:GLY:O	2.06	0.74
2:B:437:COA:O6A	2:B:437:COA:OAP	1.97	0.73
1:B:197:LEU:C	1:B:197:LEU:HD23	2.14	0.73
1:A:316:ARG:HG2	1:A:317:SER:H	1.54	0.72
1:B:307:LEU:HD22	1:B:312:ILE:HG21	1.71	0.72
1:B:270:GLU:OE2	1:B:277:ILE:O	2.08	0.71
1:A:286:PHE:O	1:A:287:VAL:HB	1.90	0.71
1:A:314:LEU:CD1	1:A:315:HIS:H	2.04	0.70
1:A:197:LEU:HD23	1:A:197:LEU:C	2.17	0.69
1:B:407:ALA:HB2	1:B:431:VAL:CG2	2.23	0.69
1:A:403:GLY:O	1:A:432:ARG:HG3	1.92	0.69
1:B:82:ARG:CZ	4:B:469:HOH:O	2.40	0.69
1:B:290:ARG:CZ	1:B:330:ILE:HD11	2.23	0.68
1:A:219:ALA:O	1:A:220:GLU:CB	2.37	0.68
1:B:320:TYR:OH	1:B:327:GLU:OE2	2.08	0.67
1:A:153:THR:HG21	4:A:440:HOH:O	1.94	0.66
1:B:290:ARG:NH1	1:B:332:GLU:OE1	2.27	0.66
1:B:215:ASP:HB2	4:B:446:HOH:O	1.94	0.66
1:B:318:ARG:HE	1:B:319:GLU:N	1.93	0.65
1:B:318:ARG:O	1:B:319:GLU:OE1	2.14	0.65
1:A:26:LEU:C	1:A:26:LEU:HD23	2.21	0.65
1:A:103:ARG:HH21	1:A:127:SER:HB2	1.61	0.65
1:A:275:ASN:O	4:A:449:HOH:O	2.15	0.64
2:A:437:COA:C2P	2:A:437:COA:O5P	2.46	0.63
1:B:209:ASP:O	1:B:278:GLY:HA2	1.99	0.63
1:A:31:ASP:OD2	1:A:33:ARG:HD3	1.99	0.63
1:A:297:ILE:HG23	1:A:321:LEU:HD13	1.81	0.63
1:A:316:ARG:HG2	1:A:317:SER:N	2.13	0.63
1:A:193:VAL:O	1:A:197:LEU:HD22	1.99	0.63
1:A:314:LEU:HD13	1:A:315:HIS:N	2.13	0.62
1:B:42:LYS:NZ	1:B:264:ASP:HB3	2.15	0.62
1:A:58:VAL:CG1	1:A:170:MET:HE2	2.29	0.62
1:A:357:LEU:O	2:A:437:COA:H21	1.99	0.62
1:A:320:TYR:C	1:A:320:TYR:CD2	2.79	0.61
1:B:316:ARG:CG	1:B:317:SER:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:CD1	4:B:482:HOH:O	2.47	0.61
1:A:286:PHE:O	1:A:287:VAL:CB	2.49	0.61
1:B:158:LEU:HD21	1:B:170:MET:HE2	1.82	0.61
1:A:33:ARG:NH2	1:A:207:LEU:HD22	2.15	0.60
1:A:21:MET:O	1:A:24:THR:HB	2.02	0.60
1:A:70:LEU:O	1:A:74:GLN:HG2	2.02	0.60
1:A:58:VAL:HG13	1:A:170:MET:HE2	1.83	0.60
1:A:270:GLU:OE2	1:A:270:GLU:HA	2.01	0.60
1:A:80:TYR:CE2	1:A:85:ARG:HB2	2.36	0.59
1:B:16:PRO:O	1:B:20:GLN:HG3	2.02	0.59
1:A:307:LEU:O	1:A:312:ILE:HD12	2.03	0.58
1:B:370:GLU:OE2	1:B:402:ARG:HD2	2.03	0.58
1:A:33:ARG:HD2	1:A:65:HIS:CG	2.38	0.58
1:B:354:ILE:HD12	1:B:376:ILE:CG1	2.33	0.58
1:B:384:GLY:O	1:B:385:ILE:HB	2.05	0.57
1:B:287:VAL:HA	1:B:332:GLU:O	2.04	0.57
1:A:315:HIS:N	1:A:315:HIS:ND1	2.51	0.57
1:A:387:ARG:HD2	1:A:433:ARG:HH11	1.67	0.57
1:B:398:TRP:CD1	1:B:402:ARG:NH2	2.72	0.57
1:B:277:ILE:HD12	1:B:277:ILE:H	1.68	0.57
1:B:307:LEU:HB3	1:B:312:ILE:HB	1.86	0.57
1:A:319:GLU:HB2	1:A:322:GLU:HG2	1.86	0.56
1:A:12:ARG:HG3	1:A:12:ARG:NH1	2.17	0.56
1:A:254:HIS:HB3	4:A:498:HOH:O	2.05	0.56
1:B:197:LEU:HD22	1:B:197:LEU:H	1.71	0.56
1:B:307:LEU:HD22	1:B:312:ILE:CG2	2.35	0.56
2:A:437:COA:HN8	2:A:437:COA:CDP	2.16	0.55
1:A:389:PHE:CD1	1:A:431:VAL:CG2	2.90	0.55
1:B:87:THR:HG23	1:B:91:SER:HB3	1.89	0.55
1:B:316:ARG:CG	1:B:317:SER:N	2.68	0.55
1:A:15:ALA:HA	1:A:18:ILE:HD12	1.90	0.54
2:B:437:COA:O5P	2:B:437:COA:C2P	2.55	0.54
1:B:290:ARG:NH2	1:B:296:ASP:OD2	2.41	0.54
1:A:353:GLU:OE1	1:A:416:ARG:HD3	2.08	0.54
2:A:437:COA:O6A	2:A:437:COA:OAP	2.20	0.53
1:A:270:GLU:OE2	1:A:277:ILE:O	2.27	0.53
1:A:213:ARG:HB3	1:A:215:ASP:OD2	2.08	0.53
1:B:19:ARG:HH11	1:B:19:ARG:CG	2.21	0.53
1:A:103:ARG:NH2	1:A:127:SER:HB2	2.23	0.52
1:A:197:LEU:HD22	1:A:197:LEU:H	1.74	0.52
1:A:17:TYR:O	1:A:21:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:SER:O	1:A:318:ARG:HG3	2.09	0.52
1:B:119:ARG:NH1	1:B:119:ARG:CG	2.57	0.52
1:A:58:VAL:CG1	1:A:170:MET:CE	2.88	0.52
2:A:437:COA:O5P	2:A:437:COA:H21	2.08	0.52
1:B:305:ARG:CB	1:B:306:PRO:CD	2.88	0.52
1:B:395:THR:HG22	1:B:395:THR:O	2.09	0.52
1:A:386:SER:C	1:A:434:LEU:HB2	2.35	0.51
1:B:319:GLU:HB2	1:B:322:GLU:H	1.74	0.51
1:A:389:PHE:CD1	1:A:431:VAL:HG22	2.46	0.50
1:B:266:SER:O	1:B:277:ILE:HD11	2.11	0.50
1:A:318:ARG:O	1:A:319:GLU:CD	2.54	0.50
1:B:364:GLN:NE2	2:B:437:COA:O9P	2.45	0.50
1:A:350:ASP:HA	1:A:385:ILE:HA	1.94	0.50
1:A:115:SER:OG	1:A:116:GLY:N	2.44	0.50
1:A:412:LEU:HD21	1:A:429:ILE:CD1	2.39	0.50
1:B:19:ARG:HH11	1:B:19:ARG:HG3	1.77	0.49
1:B:427:SER:N	4:B:539:HOH:O	2.30	0.49
1:A:30:ILE:HG12	1:A:205:LEU:HD12	1.95	0.49
1:B:402:ARG:HG3	4:B:480:HOH:O	2.13	0.49
1:A:35:LEU:HD13	1:A:102:VAL:CG1	2.43	0.49
1:B:236:SER:O	1:B:240:ARG:HG3	2.12	0.49
2:B:437:COA:HN8	2:B:437:COA:CDP	2.22	0.49
1:B:290:ARG:HH22	1:B:296:ASP:CG	2.21	0.49
1:A:307:LEU:HD22	2:A:437:COA:H61	1.94	0.48
1:B:429:ILE:C	1:B:429:ILE:HD12	2.37	0.48
1:B:31:ASP:OD1	1:B:33:ARG:NH1	2.47	0.48
1:B:312:ILE:HG23	4:B:542:HOH:O	2.12	0.48
1:A:15:ALA:HB3	1:A:16:PRO:HD3	1.95	0.48
1:B:393:THR:HB	1:B:427:SER:OG	2.13	0.48
1:B:42:LYS:HZ1	1:B:264:ASP:HB3	1.77	0.47
1:B:305:ARG:CB	1:B:306:PRO:HD3	2.45	0.47
1:B:376:ILE:C	1:B:376:ILE:HD12	2.39	0.47
1:A:26:LEU:C	1:A:26:LEU:CD2	2.86	0.47
1:B:33:ARG:HD2	1:B:65:HIS:CB	2.44	0.47
1:B:394:ASN:HD22	1:B:395:THR:N	2.12	0.47
1:A:33:ARG:CZ	1:A:207:LEU:HD22	2.45	0.47
1:B:213:ARG:C	1:B:215:ASP:H	2.22	0.46
1:B:406:THR:HA	1:B:430:LEU:HD23	1.97	0.46
1:A:35:LEU:HD13	1:A:102:VAL:HG11	1.98	0.46
1:B:42:LYS:HZ3	1:B:264:ASP:HB3	1.81	0.46
1:A:365:ASP:OD2	2:A:437:COA:H3B	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ALA:CB	1:B:431:VAL:CG2	2.93	0.46
1:B:427:SER:HB2	4:B:539:HOH:O	2.16	0.46
1:B:82:ARG:NE	4:B:469:HOH:O	2.46	0.46
1:A:389:PHE:CD1	1:A:431:VAL:HG21	2.50	0.46
1:B:318:ARG:HH21	1:B:319:GLU:HA	1.80	0.46
2:A:437:COA:H131	2:A:437:COA:N8P	2.20	0.46
1:B:317:SER:O	1:B:318:ARG:O	2.32	0.46
1:B:30:ILE:HG12	1:B:205:LEU:HD12	1.98	0.45
1:B:305:ARG:HB2	1:B:306:PRO:CD	2.45	0.45
1:A:419:ASP:C	1:A:421:ARG:H	2.24	0.45
1:A:249:LEU:HD21	1:A:256:VAL:HG12	1.99	0.45
1:B:236:SER:HA	1:B:239:ARG:HB3	1.99	0.45
1:B:318:ARG:HE	1:B:319:GLU:CA	2.29	0.45
1:A:332:GLU:HA	1:A:336:ASN:O	2.17	0.45
1:B:124:PRO:HB2	1:B:166:ASN:ND2	2.32	0.45
1:A:317:SER:C	1:A:318:ARG:HG3	2.41	0.45
1:B:211:ILE:CD1	1:B:258:ILE:HG13	2.47	0.45
1:A:60:ILE:HG12	1:A:170:MET:HB2	2.00	0.44
1:A:242:ILE:O	1:A:243:SER:C	2.61	0.44
1:A:263:ALA:HB3	1:A:266:SER:OG	2.18	0.44
1:A:303:LEU:HB3	1:A:304:ILE:HD12	1.99	0.44
1:B:124:PRO:HB2	1:B:166:ASN:HD22	1.83	0.44
1:A:220:GLU:HA	1:A:278:GLY:O	2.18	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.84	0.43
1:A:407:ALA:CB	4:A:439:HOH:O	2.52	0.43
1:B:155:THR:HG22	1:B:159:ARG:NH1	2.33	0.43
2:B:437:COA:O5P	2:B:437:COA:N8P	2.51	0.43
1:B:211:ILE:HD12	1:B:258:ILE:HG13	2.01	0.43
1:B:286:PHE:O	1:B:287:VAL:CB	2.66	0.43
1:B:318:ARG:HE	1:B:318:ARG:C	2.25	0.43
1:B:17:TYR:O	1:B:21:MET:HG2	2.18	0.43
1:B:286:PHE:O	1:B:287:VAL:HB	2.18	0.43
1:B:364:GLN:CD	4:B:543:HOH:O	2.61	0.43
1:B:416:ARG:HD2	1:B:416:ARG:HA	1.78	0.43
1:A:126:VAL:HG11	1:A:161:GLN:NE2	2.34	0.43
1:A:213:ARG:C	1:A:215:ASP:N	2.77	0.43
1:A:50:LEU:HD11	1:A:267:LEU:HD13	2.01	0.42
1:A:277:ILE:O	1:A:277:ILE:HD12	2.19	0.42
2:B:437:COA:O5P	2:B:437:COA:H21	2.19	0.42
1:A:56:ARG:HB3	1:A:162:LEU:HD22	2.01	0.42
1:A:394:ASN:HD22	1:A:395:THR:N	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ASP:HA	4:A:443:HOH:O	2.18	0.42
1:B:213:ARG:O	1:B:215:ASP:N	2.52	0.42
1:A:180:LYS:HA	1:A:180:LYS:HD3	1.88	0.42
1:B:305:ARG:HB2	1:B:306:PRO:HD3	2.01	0.42
1:A:420:TYR:O	1:A:426:ASN:OD1	2.38	0.42
1:B:426:ASN:HB2	4:B:455:HOH:O	2.19	0.42
1:A:324:HIS:O	1:A:327:GLU:HG2	2.20	0.42
1:B:200:GLU:O	1:B:254:HIS:HB2	2.20	0.42
1:A:213:ARG:C	1:A:215:ASP:H	2.27	0.42
1:B:384:GLY:O	1:B:385:ILE:CB	2.66	0.42
1:B:213:ARG:HB3	1:B:214:PRO:HD2	2.00	0.41
1:B:197:LEU:HD22	1:B:197:LEU:N	2.33	0.41
1:A:231:ALA:HB1	1:A:239:ARG:NH1	2.34	0.41
1:A:77:THR:HA	1:A:78:PRO:HD2	1.88	0.41
1:A:104:SER:OG	1:B:96:GLN:HG2	2.19	0.41
1:B:418:LYS:HA	1:B:418:LYS:HD2	1.87	0.41
1:B:412:LEU:HD23	1:B:412:LEU:HA	1.91	0.41
1:A:386:SER:O	1:A:434:LEU:N	2.52	0.41
1:B:373:LEU:O	1:B:377:ILE:HG23	2.20	0.41
1:A:299:HIS:CB	1:A:337:LEU:HD12	2.51	0.41
1:A:418:LYS:O	1:A:421:ARG:HG2	2.20	0.41
1:B:318:ARG:C	1:B:319:GLU:HG2	2.46	0.41
1:A:286:PHE:HD2	1:A:334:ASP:HB2	1.86	0.41
1:B:333:HIS:HE1	4:B:448:HOH:O	2.03	0.41
1:B:337:LEU:N	1:B:337:LEU:HD23	2.36	0.41
1:B:427:SER:HB3	1:B:428:HIS:H	1.65	0.41
1:A:197:LEU:O	1:A:198:GLN:C	2.64	0.40
1:B:290:ARG:NH2	1:B:330:ILE:HD11	2.36	0.40
1:A:386:SER:HA	1:A:434:LEU:HB2	2.02	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	A	418/456 (92%)	383 (92%)	27 (6%)	8 (2%)	6	7
1	B	418/456 (92%)	395 (94%)	13 (3%)	10 (2%)	4	4
All	All	836/912 (92%)	778 (93%)	40 (5%)	18 (2%)	5	5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	GLU
1	B	219	ALA
1	B	220	GLU
1	B	318	ARG
1	A	318	ARG
1	A	420	TYR
1	B	306	PRO
1	B	314	LEU
1	A	411	GLU
1	B	63	ALA
1	B	385	ILE
1	A	287	VAL
1	B	214	PRO
1	B	287	VAL
1	B	414	GLU
1	A	410	ASP
1	A	214	PRO
1	A	295	GLY

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	A	329/355 (93%)	288 (88%)	41 (12%)	4	4
1	B	329/355 (93%)	278 (84%)	51 (16%)	2	2
All	All	658/710 (93%)	566 (86%)	92 (14%)	3	3

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	24	THR
1	A	26	LEU
1	A	40	LEU
1	A	47	ILE
1	A	49	LEU
1	A	70	LEU
1	A	101	THR
1	A	105	ARG
1	A	119	ARG
1	A	132	THR
1	A	140	ASP
1	A	153	THR
1	A	197	LEU
1	A	225	GLN
1	A	230	LEU
1	A	238	THR
1	A	250	GLU
1	A	256	VAL
1	A	277	ILE
1	A	290	ARG
1	A	303	LEU
1	A	304	ILE
1	A	312	ILE
1	A	313	LEU
1	A	315	HIS
1	A	316	ARG
1	A	317	SER
1	A	318	ARG
1	A	320	TYR
1	A	321	LEU
1	A	330	ILE
1	A	383	ILE
1	A	388	LEU
1	A	394	ASN
1	A	395	THR
1	A	402	ARG
1	A	411	GLU
1	A	414	GLU
1	A	421	ARG
1	A	429	ILE
1	B	19	ARG
1	B	24	THR

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Mol	Chain	Res	Type
1	B	33	ARG
1	B	40	LEU
1	B	42	LYS
1	B	70	LEU
1	B	76	ARG
1	B	84	LEU
1	B	92	LEU
1	B	101	THR
1	B	105	ARG
1	B	114	VAL
1	B	119	ARG
1	B	126	VAL
1	B	132	THR
1	B	149	VAL
1	B	153	THR
1	B	197	LEU
1	B	215	ASP
1	B	238	THR
1	B	244	SER
1	B	250	GLU
1	B	256	VAL
1	B	259	LEU
1	B	264	ASP
1	B	266	SER
1	B	268	LEU
1	B	277	ILE
1	B	291	GLN
1	B	304	ILE
1	B	312	ILE
1	B	313	LEU
1	B	314	LEU
1	B	316	ARG
1	B	317	SER
1	B	318	ARG
1	B	321	LEU
1	B	330	ILE
1	B	337	LEU
1	B	370	GLU
1	B	377	ILE
1	B	381	ARG
1	B	386	SER
1	B	394	ASN

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Mol	Chain	Res	Type
1	B	397	GLU
1	B	402	ARG
1	B	406	THR
1	B	414	GLU
1	B	421	ARG
1	B	429	ILE
1	B	431	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	161	GLN
1	A	225	GLN
1	A	364	GLN
1	A	394	ASN
1	A	426	ASN
1	B	74	GLN
1	B	94	GLN
1	B	161	GLN
1	B	166	ASN
1	B	275	ASN
1	B	333	HIS
1	B	364	GLN
1	B	394	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

4 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	COA	A	437	-	47,50,50	1.98	9 (19%)	69,75,75	1.81	16 (23%)
2	COA	B	437	-	47,50,50	1.73	8 (17%)	69,75,75	1.92	21 (30%)
3	ARG	A	438	-	10,11,11	0.92	1 (10%)	9,13,13	1.16	1 (11%)
3	ARG	B	438	-	10,11,11	0.74	0	9,13,13	0.88	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	COA	A	437	-	1/1/11/13	14/48/64/64	0/3/3/3
2	COA	B	437	-	1/1/11/13	13/48/64/64	0/3/3/3
3	ARG	A	438	-	-	1/11/11/11	-
3	ARG	B	438	-	-	0/11/11/11	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	437	COA	P3B-O7A	5.69	1.68	1.50
2	A	437	COA	P2A-O3A	5.60	1.65	1.59
2	A	437	COA	C3P-N4P	-5.08	1.34	1.46
2	B	437	COA	P3B-O7A	5.02	1.66	1.50
2	B	437	COA	C3P-N4P	-4.69	1.35	1.46
2	A	437	COA	P1A-O3A	4.65	1.64	1.59
2	B	437	COA	P3B-O8A	4.09	1.70	1.54
2	A	437	COA	P3B-O8A	3.74	1.68	1.54
2	B	437	COA	P2A-O3A	-3.42	1.55	1.59
2	A	437	COA	P3B-O3B	2.75	1.64	1.59
2	B	437	COA	C5A-N7A	-2.64	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	437	COA	O4B-C1B	2.64	1.48	1.42
2	A	437	COA	C8A-N7A	2.54	1.36	1.31
2	A	437	COA	C5B-C4B	2.52	1.59	1.51
2	B	437	COA	C8A-N9A	-2.47	1.33	1.37
3	A	438	ARG	OXT-C	-2.42	1.22	1.30
2	A	437	COA	CCP-CBP	2.13	1.56	1.52
2	B	437	COA	C8A-N7A	2.04	1.35	1.31

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	437	COA	C5A-C4A-N3A	-4.92	119.94	126.72
2	A	437	COA	C5A-C4A-N3A	-4.84	120.05	126.72
2	A	437	COA	N3A-C2A-N1A	-4.75	121.39	128.58
2	B	437	COA	C2P-C3P-N4P	4.21	121.86	112.31
2	B	437	COA	N3A-C2A-N1A	-4.20	122.22	128.58
2	A	437	COA	C7P-N8P-C9P	-4.10	115.18	122.55
2	B	437	COA	N9A-C8A-N7A	-3.85	108.48	113.94
2	A	437	COA	C2A-N3A-C4A	3.61	120.64	111.83
2	B	437	COA	C4A-C5A-N7A	-3.57	106.50	110.58
2	A	437	COA	CEP-CBP-CCP	3.49	113.98	108.22
2	B	437	COA	C2A-N3A-C4A	3.33	119.96	111.83
2	B	437	COA	C7P-N8P-C9P	-3.26	116.69	122.55
2	B	437	COA	C5A-N7A-C8A	3.25	108.55	103.45
2	A	437	COA	N9A-C8A-N7A	-3.22	109.37	113.94
2	A	437	COA	N3A-C4A-N9A	3.16	132.55	127.17
3	A	438	ARG	OXT-C-O	-3.15	116.92	124.08
2	B	437	COA	N3A-C4A-N9A	3.14	132.51	127.17
2	B	437	COA	C4A-N9A-C8A	3.03	108.92	105.74
2	B	437	COA	CEP-CBP-CCP	3.01	113.19	108.22
2	A	437	COA	C2P-C3P-N4P	2.82	118.70	112.31
2	A	437	COA	CDP-CBP-CAP	2.77	113.49	108.77
2	B	437	COA	O4B-C1B-N9A	2.64	113.16	108.09
2	B	437	COA	O9P-C9P-CAP	-2.52	113.87	120.89
2	B	437	COA	O3A-P1A-O1A	-2.51	103.17	110.70
2	B	437	COA	C6P-C7P-N8P	2.45	117.22	112.00
2	B	437	COA	P3B-O3B-C3B	-2.42	116.97	123.43
2	B	437	COA	O9A-P3B-O8A	2.38	116.73	107.80
2	A	437	COA	C5A-N7A-C8A	2.37	107.18	103.45
2	A	437	COA	O5P-C5P-C6P	-2.35	117.76	122.02
2	B	437	COA	O8A-P3B-O7A	-2.35	101.69	110.83
2	A	437	COA	C4A-C5A-N7A	-2.34	107.91	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	437	COA	C4A-N9A-C8A	2.28	108.14	105.74
2	B	437	COA	O5P-C5P-C6P	-2.18	118.07	122.02
2	A	437	COA	O3A-P1A-O1A	-2.16	104.22	110.70
2	B	437	COA	CDP-CBP-CAP	2.15	112.44	108.77
2	B	437	COA	O2A-P1A-O1A	2.09	122.18	112.44
2	A	437	COA	O2A-P1A-O3A	2.09	112.93	107.27
2	A	437	COA	O5P-C5P-N4P	2.00	126.96	123.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	437	COA	CAP
2	B	437	COA	CAP

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	437	COA	C5B-O5B-P1A-O2A
2	A	437	COA	C5B-O5B-P1A-O3A
2	A	437	COA	CCP-O6A-P2A-O4A
2	A	437	COA	O9P-C9P-CAP-CBP
2	A	437	COA	N8P-C9P-CAP-CBP
2	A	437	COA	C2P-C3P-N4P-C5P
2	B	437	COA	C5B-O5B-P1A-O2A
2	B	437	COA	C5B-O5B-P1A-O3A
2	B	437	COA	O9P-C9P-CAP-CBP
2	B	437	COA	N8P-C9P-CAP-CBP
2	B	437	COA	C2P-C3P-N4P-C5P
2	A	437	COA	O9P-C9P-CAP-OAP
2	B	437	COA	O9P-C9P-CAP-OAP
2	A	437	COA	C5B-O5B-P1A-O1A
2	A	437	COA	CCP-O6A-P2A-O3A
2	A	437	COA	CCP-O6A-P2A-O5A
2	B	437	COA	C5B-O5B-P1A-O1A
2	B	437	COA	CCP-O6A-P2A-O3A
2	B	437	COA	CCP-O6A-P2A-O4A
2	B	437	COA	CCP-O6A-P2A-O5A
3	A	438	ARG	NE-CD-CG-CB
2	A	437	COA	P2A-O3A-P1A-O1A
2	A	437	COA	C2B-C1B-N9A-C8A
2	A	437	COA	P2A-O3A-P1A-O2A
2	B	437	COA	P2A-O3A-P1A-O2A

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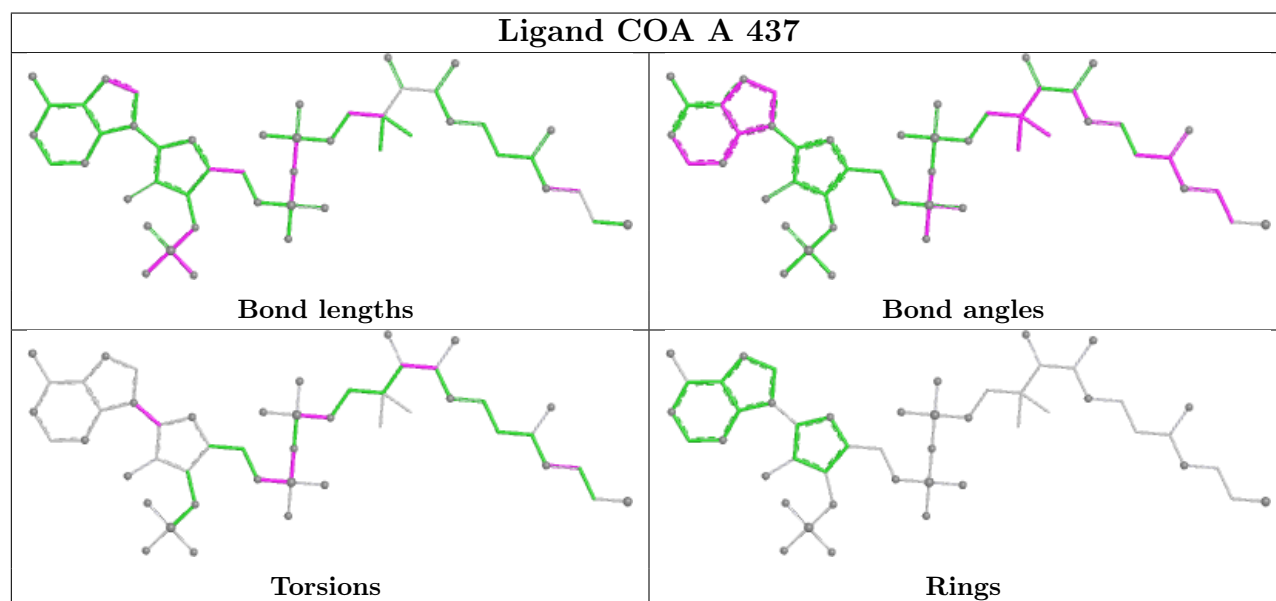
Mol	Chain	Res	Type	Atoms
2	B	437	COA	C2B-C1B-N9A-C8A
2	A	437	COA	N8P-C9P-CAP-OAP
2	B	437	COA	N8P-C9P-CAP-OAP

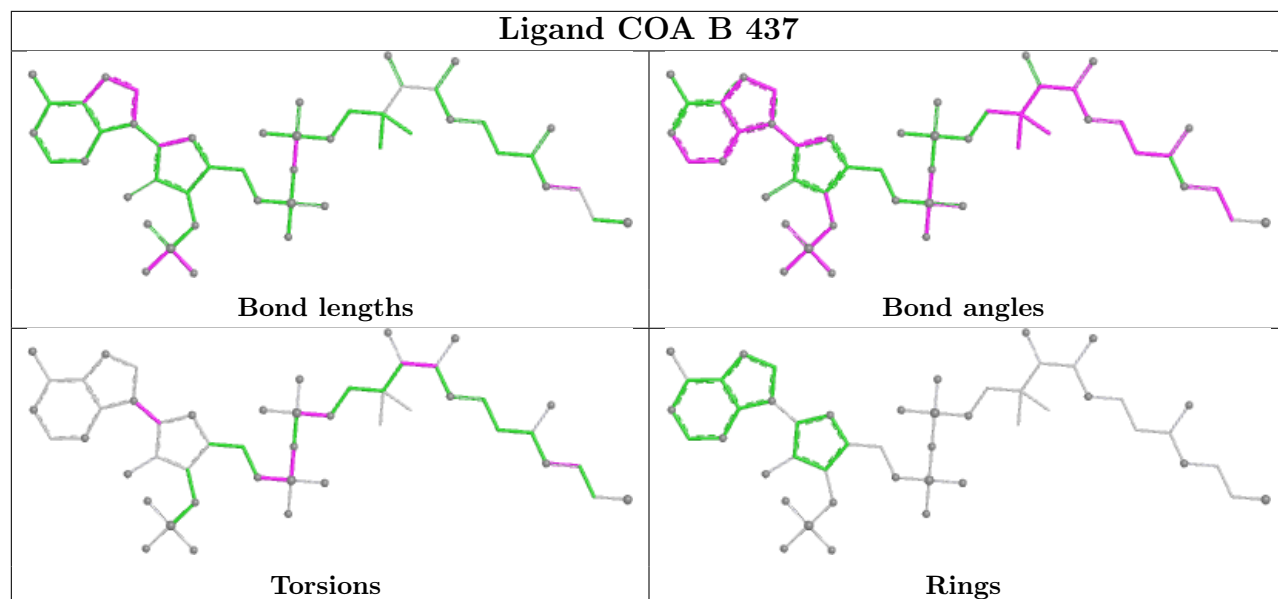
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	437	COA	9	0
2	B	437	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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	424/456 (92%)	0.23	20 (4%) 36 37	21, 29, 35, 42	0
1	B	424/456 (92%)	-0.06	16 (3%) 44 45	19, 28, 35, 41	0
All	All	848/912 (92%)	0.08	36 (4%) 40 41	19, 29, 35, 42	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	LEU	6.8
1	B	302	ALA	5.7
1	A	410	ASP	4.4
1	B	318	ARG	4.1
1	A	214	PRO	3.5
1	B	312	ILE	3.5
1	B	84	LEU	3.5
1	A	314	LEU	3.3
1	A	412	LEU	3.3
1	B	315	HIS	3.2
1	A	351	CYS	3.2
1	B	317	SER	3.1
1	A	317	SER	3.0
1	A	313	LEU	3.0
1	A	318	ARG	3.0
1	A	303	LEU	2.9
1	B	304	ILE	2.9
1	A	409	GLU	2.8
1	A	426	ASN	2.6
1	A	302	ALA	2.6
1	A	421	ARG	2.5
1	A	363	ALA	2.4
1	A	312	ILE	2.4
1	B	307	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	313	LEU	2.4
1	B	435	HIS	2.4
1	B	314	LEU	2.3
1	B	79	HIS	2.3
1	A	434	LEU	2.3
1	A	407	ALA	2.3
1	B	239	ARG	2.3
1	B	436	ARG	2.2
1	A	393	THR	2.2
1	A	408	SER	2.2
1	B	319	GLU	2.1
1	A	221	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

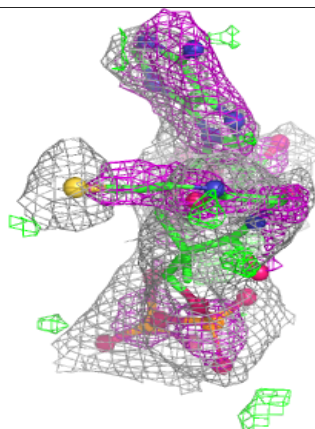
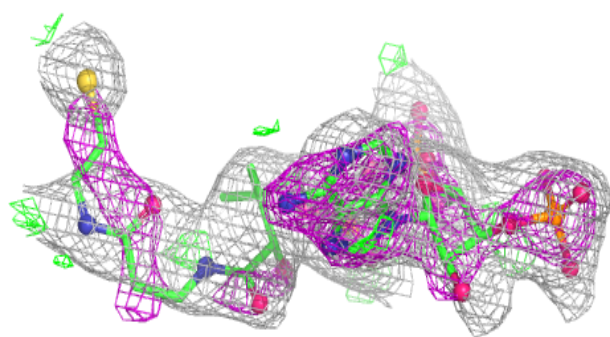
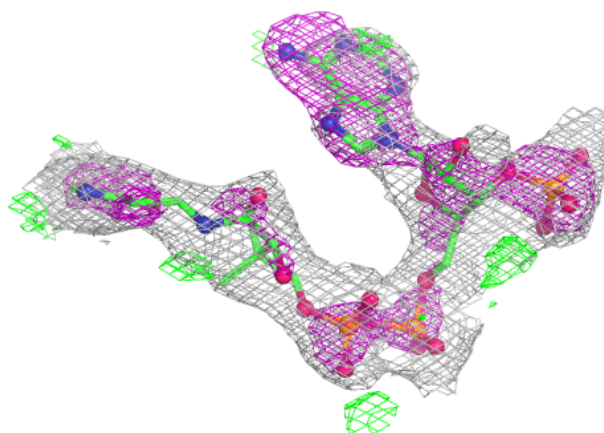
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	COA	A	437	48/48	0.82	0.14	34,42,47,57	0
2	COA	B	437	48/48	0.84	0.13	34,42,47,58	0
3	ARG	A	438	12/12	0.95	0.12	28,32,33,33	0
3	ARG	B	438	12/12	0.95	0.10	26,32,34,35	0

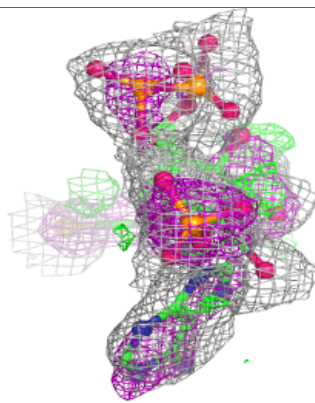
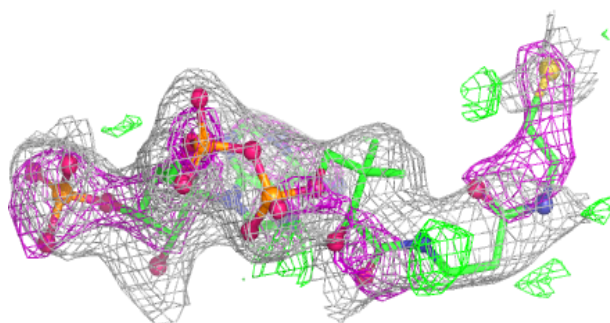
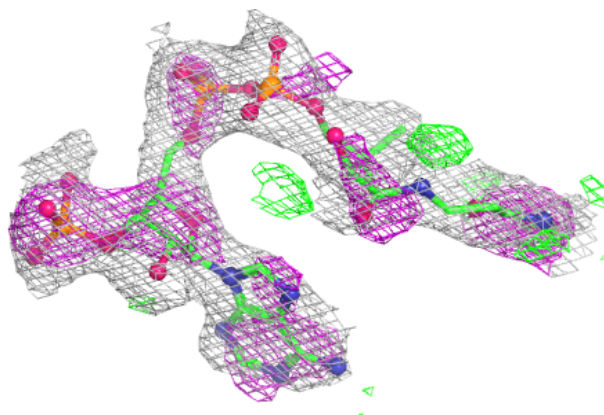
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA A 437:

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

**Electron density around COA B 437:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.