



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 04:50 pm GMT

PDB ID : 3D2P  
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](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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

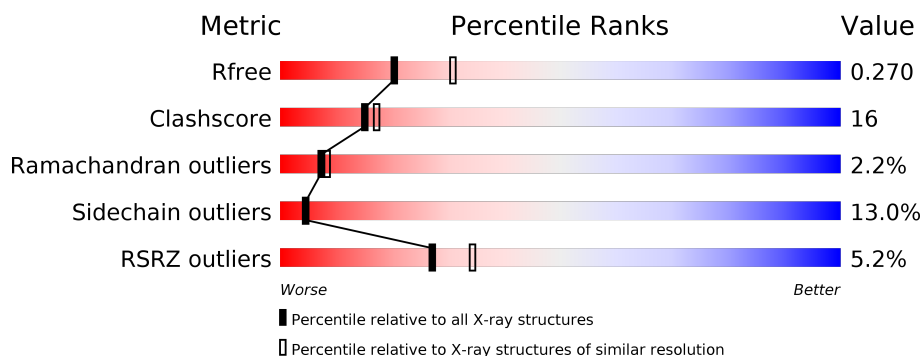
# 1 Overall quality at a glance

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))
$R_{free}$	111664	1056 (2.58-2.54)
Clashscore	122126	1102 (2.58-2.54)
Ramachandran outliers	120053	1092 (2.58-2.54)
Sidechain outliers	120020	1092 (2.58-2.54)
RSRZ outliers	108989	1048 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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:

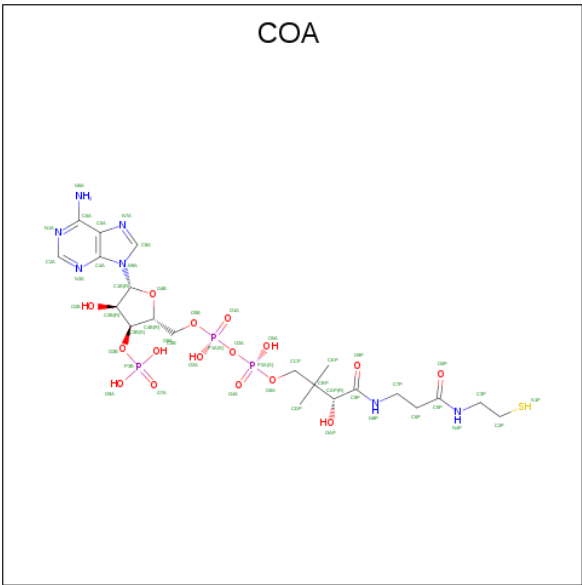
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q5FAK7
A	-18	GLY	-	EXPRESSION TAG	UNP Q5FAK7
A	-17	SER	-	EXPRESSION TAG	UNP Q5FAK7
A	-16	SER	-	EXPRESSION TAG	UNP Q5FAK7
A	-15	HIS	-	EXPRESSION TAG	UNP Q5FAK7
A	-14	HIS	-	EXPRESSION TAG	UNP Q5FAK7
A	-13	HIS	-	EXPRESSION TAG	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	UNP Q5FAK7
A	336	ASN	ASP	ENGINEERED	UNP Q5FAK7
A	427	SER	PRO	ENGINEERED	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	UNP Q5FAK7
B	336	ASN	ASP	ENGINEERED	UNP Q5FAK7
B	427	SER	PRO	ENGINEERED	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).



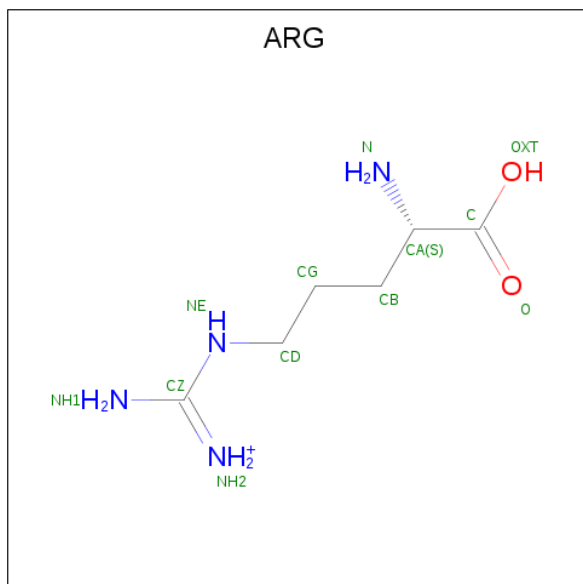
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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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 (three-letter code: 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, $\alpha$ , $\beta$ , $\gamma$	107.05Å 107.05Å 185.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.56 44.97 – 2.56	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-2.56) 90.8 (44.97-2.56)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6745	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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

### 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	0.84	5/3277 (0.2%)	0.94	8/4430 (0.2%)
1	B	0.84	2/3277 (0.1%)	0.91	5/4430 (0.1%)
All	All	0.84	7/6554 (0.1%)	0.93	13/8860 (0.1%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	ARG	NE-CZ	16.47	1.54	1.33
1	A	387	ARG	CZ-NH1	15.89	1.53	1.33
1	B	81	CYS	CB-SG	-9.65	1.65	1.82
1	A	350	ASP	C-N	8.13	1.52	1.34
1	A	433	ARG	CZ-NH1	5.67	1.40	1.33
1	B	111	CYS	CB-SG	-5.45	1.73	1.81
1	A	319	GLU	CB-CG	5.17	1.61	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	ARG	NE-CZ-NH1	-20.91	109.84	120.30
1	A	433	ARG	NE-CZ-NH2	-11.51	114.55	120.30
1	A	433	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	387	ARG	NE-CZ-NH2	-9.40	115.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	LEU	CB-CG-CD2	-7.37	98.47	111.00
1	A	313	LEU	CA-CB-CG	7.34	132.18	115.30
1	B	22	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	22	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	313	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	387	ARG	CD-NE-CZ	-6.02	115.17	123.60
1	A	92	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	277	ILE	N-CA-C	-5.72	95.56	111.00
1	A	277	ILE	N-CA-C	-5.17	97.03	111.00

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

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	98	0
1	B	3223	0	3213	101	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	14	0
All	All	6745	0	6514	210	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 16.

All (210) 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:HH11	1:A:119:ARG:HG2	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:NH1	1:B:119:ARG:HG2	1.73	0.95
1:A:119:ARG:NH1	1:A:119:ARG:HG2	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:H131	2:A:437:COA:HN8	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
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: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: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:B:318:ARG:O	1:B:319:GLU:CD	2.30	0.70
1:A:314:LEU:CD1	1:A:315:HIS:H	2.04	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:C	1:B:197:LEU:HD23	2.14	0.68
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:103:ARG:HH21	1:A:127:SER:HB2	1.61	0.65
1:A:197:LEU:C	1:A:197:LEU:HD23	2.17	0.64
1:A:275:ASN:O	4:A:449:HOH:O	2.15	0.64
2:A:437:COA:O5P	2:A:437:COA:C2P	2.46	0.63
1:B:209:ASP:O	1:B:278:GLY:HA2	1.99	0.63
1:A:297:ILE:HG23	1:A:321:LEU:HD13	1.81	0.63
1:A:31:ASP:OD2	1:A:33:ARG:HD3	1.99	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:357:LEU:O	2:A:437:COA:H21	1.99	0.62
1:B:316:ARG:CG	1:B:317:SER:H	2.09	0.61
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: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:26:LEU:HD23	1:A:26:LEU:C	2.21	0.60
1:A:270:GLU:HA	1:A:270:GLU:OE2	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:ND1	1:A:315:HIS:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LEU:HB3	1:B:312:ILE:HB	1.86	0.57
1:A:320:TYR:CD2	1:A:320:TYR:C	2.79	0.56
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:H	1:B:197:LEU:HD22	1.71	0.56
1:B:307:LEU:HD22	1:B:312:ILE:CG2	2.35	0.56
2:A:437:COA:CDP	2:A:437:COA:HN8	2.16	0.55
1:A:389:PHE:CD1	1:A:431:VAL:CG2	2.90	0.55
1:B:316:ARG:CG	1:B:317:SER:N	2.68	0.55
1:B:87:THR:HG23	1:B:91:SER:HB3	1.89	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
1:A:60:ILE:HD11	1:A:170:MET:HE1	1.90	0.54
2:A:437:COA:OAP	2:A:437:COA:O6A	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:CG	1:B:19:ARG:HH11	2.21	0.53
1:A:103:ARG:NH2	1:A:127:SER:HB2	2.23	0.52
1:A:197:LEU:H	1:A:197:LEU:HD22	1.74	0.52
1:A:17:TYR:O	1:A:21:MET:HG2	2.09	0.52
1:A:317:SER:O	1:A:318:ARG:HG3	2.09	0.52
1:B:119:ARG:CG	1:B:119:ARG:NH1	2.57	0.52
1:A:58:VAL:CG1	1:A:170:MET:CE	2.88	0.52
2:A:437:COA:H21	2:A:437:COA:O5P	2.08	0.52
1:B:305:ARG:CB	1:B:306:PRO:CD	2.88	0.52
1:B:395:THR:O	1:B:395:THR:HG22	2.09	0.52
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:SER:O	1:B:240:ARG:HG3	2.12	0.49
2:B:437:COA:CDP	2:B:437:COA:HN8	2.22	0.49
1:A:307:LEU:HD22	2:A:437:COA:H61	1.94	0.48
1:B:312:ILE:HG23	4:B:542:HOH:O	2.12	0.48
1:B:31:ASP:OD1	1:B:33:ARG:NH1	2.47	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:HZ3	1:B:264:ASP:HB3	1.79	0.47
1:B:305:ARG:CB	1:B:306:PRO:HD3	2.45	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:A:386:SER:C	1:A:434:LEU:HB2	2.35	0.47
1:A:58:VAL:CG1	1:A:170:MET:HE2	2.45	0.47
1:B:406:THR:HA	1:B:430:LEU:HD23	1.97	0.46
1:B:42:LYS:HZ1	1:B:264:ASP:HB3	1.78	0.46
1:A:35:LEU:HD13	1:A:102:VAL:HG11	1.98	0.46
1:A:365:ASP:OD2	2:A:437:COA:H3B	2.15	0.46
1:B:427:SER:HB2	4:B:539:HOH:O	2.16	0.46
1:B:407:ALA:CB	1:B:431:VAL:CG2	2.93	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:305:ARG:HB2	1:B:306:PRO:CD	2.45	0.45
1:B:30:ILE:HG12	1:B:205:LEU:HD12	1.98	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: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:318:ARG:O	1:A:319:GLU:CD	2.54	0.44
1:B:290:ARG:HH22	1:B:296:ASP:CG	2.21	0.44
1:A:263:ALA:HB3	1:A:266:SER:OG	2.18	0.44
1:B:429:ILE:C	1:B:429:ILE:HD12	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:416:ARG:HA	1:B:416:ARG:HD2	1.78	0.43
1:A:126:VAL:HG11	1:A:161:GLN:NE2	2.34	0.43
1:B:376:ILE:C	1:B:376:ILE:HD12	2.39	0.43
1:A:50:LEU:HD11	1:A:267:LEU:HD13	2.01	0.42
1:A:26:LEU:C	1:A:26:LEU:CD2	2.86	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
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:B:213:ARG:C	1:B:215:ASP:H	2.22	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:N	1:B:197:LEU:HD22	2.33	0.41
1:A:231:ALA:HB1	1:A:239:ARG:NH1	2.34	0.41
1:A:104:SER:OG	1:B:96:GLN:HG2	2.19	0.41
1:A:77:THR:HA	1:A:78:PRO:HD2	1.88	0.41
1:B:418:LYS:HD2	1:B:418:LYS:HA	1.87	0.41
1:B:412:LEU:HA	1:B:412:LEU:HD23	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:A:286:PHE:HD2	1:A:334:ASP:HB2	1.86	0.41
1:A:419:ASP:C	1:A:421:ARG:H	2.24	0.41
1:B:333:HIS:HE1	4:B:448:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 [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	418/456 (92%)	383 (92%)	27 (6%)	8 (2%)	9	11
1	B	418/456 (92%)	395 (94%)	13 (3%)	10 (2%)	6	7
All	All	836/912 (92%)	778 (93%)	40 (5%)	18 (2%)	7	8

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

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Mol	Chain	Res	Type
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%)	294 (89%)	35 (11%)	7	8
1	B	329/355 (93%)	278 (84%)	51 (16%)	3	2
All	All	658/710 (93%)	572 (87%)	86 (13%)	4	4

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	40	LEU
1	A	49	LEU
1	A	70	LEU
1	A	81	CYS
1	A	101	THR
1	A	119	ARG
1	A	132	THR
1	A	153	THR
1	A	197	LEU
1	A	225	GLN
1	A	238	THR
1	A	250	GLU
1	A	256	VAL
1	A	264	ASP
1	A	290	ARG
1	A	303	LEU
1	A	305	ARG
1	A	313	LEU

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Mol	Chain	Res	Type
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
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	85	ARG
1	B	101	THR
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	254	HIS
1	B	256	VAL
1	B	259	LEU
1	B	264	ASP
1	B	266	SER

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Mol	Chain	Res	Type
1	B	268	LEU
1	B	277	ILE
1	B	290	ARG
1	B	291	GLN
1	B	304	ILE
1	B	312	ILE
1	B	313	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
1	B	397	GLU
1	B	406	THR
1	B	414	GLU
1	B	421	ARG
1	B	429	ILE
1	B	431	VAL
1	B	436	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	94	GLN
1	A	161	GLN
1	A	166	ASN
1	A	225	GLN
1	A	364	GLN
1	A	394	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

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Mol	Chain	Res	Type
1	B	364	GLN
1	B	394	ASN
1	B	426	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 carbohydrates 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	-	41,50,50	1.66	6 (14%)	51,75,75	2.03	11 (21%)
3	ARG	A	438	-	6,11,11	0.61	0	5,13,13	0.61	0
2	COA	B	437	-	41,50,50	1.74	6 (14%)	51,75,75	1.99	13 (25%)
3	ARG	B	438	-	6,11,11	0.26	0	5,13,13	0.64	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	1/44/64/64	0/3/3/3
3	ARG	A	438	-	-	0/7/11/11	0/0/0/0
2	COA	B	437	-	1/1/11/13	2/44/64/64	0/3/3/3
3	ARG	B	438	-	-	0/7/11/11	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	437	COA	C3P-N4P	-4.89	1.34	1.46
2	B	437	COA	C3P-N4P	-4.52	1.35	1.46
2	B	437	COA	C8A-N9A	-2.98	1.33	1.36
2	B	437	COA	C9P-N8P	2.18	1.38	1.33
2	A	437	COA	C5B-C4B	2.35	1.59	1.51
2	A	437	COA	P3B-O3B	2.67	1.64	1.59
2	A	437	COA	P3B-O8A	3.44	1.68	1.54
2	A	437	COA	O4B-C1B	3.44	1.46	1.41
2	B	437	COA	P3B-O8A	3.75	1.70	1.54
2	B	437	COA	P3B-O7A	4.60	1.66	1.50
2	B	437	COA	O4B-C1B	4.91	1.48	1.41
2	A	437	COA	P3B-O7A	5.22	1.68	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	437	COA	N3A-C2A-N1A	-8.73	121.39	128.86
2	B	437	COA	N3A-C2A-N1A	-7.76	122.22	128.86
2	A	437	COA	C4B-O4B-C1B	-4.23	105.41	109.83
2	A	437	COA	C7P-N8P-C9P	-4.04	115.18	122.59
2	A	437	COA	P2A-O3A-P1A	-3.68	120.25	132.63
2	B	437	COA	C4B-O4B-C1B	-3.66	106.02	109.83
2	B	437	COA	P2A-O3A-P1A	-3.35	121.39	132.63
2	B	437	COA	C7P-N8P-C9P	-3.21	116.69	122.59
2	B	437	COA	C4A-C5A-N7A	-3.01	106.50	109.41
2	A	437	COA	O5P-C5P-C6P	-2.29	117.76	122.00
2	B	437	COA	O8A-P3B-O7A	-2.28	101.69	110.60
2	A	437	COA	C1B-N9A-C4A	-2.25	122.75	126.64
2	B	437	COA	O9P-C9P-CAP	-2.17	113.87	120.78
2	B	437	COA	O5P-C5P-C6P	-2.12	118.07	122.00
2	A	437	COA	C6P-C7P-N8P	2.00	115.91	111.85
2	B	437	COA	CDP-CBP-CAP	2.09	112.44	108.82
2	A	437	COA	O5P-C5P-N4P	2.10	126.96	123.02
2	B	437	COA	O9A-P3B-O8A	2.31	116.73	107.59
2	B	437	COA	C6P-C7P-N8P	2.64	117.22	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	437	COA	C2P-C3P-N4P	2.69	118.70	112.33
2	A	437	COA	CDP-CBP-CAP	2.69	113.49	108.82
2	B	437	COA	CEP-CBP-CCP	3.04	113.19	108.23
2	A	437	COA	CEP-CBP-CCP	3.52	113.98	108.23
2	B	437	COA	C2P-C3P-N4P	4.02	121.86	112.33

All (2) chirality outliers are listed below:

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

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	437	COA	O9P-C9P-CAP-CBP
2	A	437	COA	C2P-C3P-N4P-C5P
2	B	437	COA	C2P-C3P-N4P-C5P

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

## 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	A	424/456 (92%)	0.26	32 (7%) 14 19	21, 29, 35, 42	0
1	B	424/456 (92%)	-0.05	12 (2%) 53 63	19, 28, 35, 41	0
All	All	848/912 (92%)	0.10	44 (5%) 27 34	19, 29, 35, 42	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	ASP	6.6
1	A	346	PHE	5.6
1	A	351	CYS	5.2
1	B	436	ARG	4.4
1	A	436	ARG	4.3
1	A	389	PHE	4.3
1	B	318	ARG	4.1
1	A	412	LEU	4.1
1	B	303	LEU	4.0
1	A	409	GLU	4.0
1	B	316	ARG	3.6
1	B	302	ALA	3.6
1	A	435	HIS	3.4
1	A	434	LEU	3.4
1	B	312	ILE	3.3
1	B	435	HIS	3.1
1	A	214	PRO	3.0
1	A	405	GLN	3.0
1	A	393	THR	3.0
1	A	388	LEU	2.9
1	A	408	SER	2.8
1	A	352	GLY	2.8
1	A	383	ILE	2.7
1	B	79	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	390	ALA	2.5
1	A	413	PRO	2.5
1	A	233	HIS	2.5
1	A	414	GLU	2.5
1	B	307	LEU	2.5
1	A	398	TRP	2.4
1	A	317	SER	2.4
1	A	313	LEU	2.4
1	B	84	LEU	2.4
1	A	421	ARG	2.3
1	A	320	TYR	2.3
1	A	387	ARG	2.2
1	A	345	THR	2.2
1	A	75	GLY	2.2
1	B	313	LEU	2.2
1	A	417	ARG	2.2
1	A	354	ILE	2.2
1	A	404	PHE	2.2
1	A	399	PHE	2.0
1	B	239	ARG	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 carbohydrates 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
2	COA	A	437	48/48	0.90	0.25	34,42,47,57	0
2	COA	B	437	48/48	0.91	0.26	34,42,47,58	0
3	ARG	A	438	12/12	0.97	0.12	28,32,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ARG	B	438	12/12	0.97	0.09	26,32,34,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.