



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:33 AM GMT

PDB ID : 2WL5  
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE  
H348N MUTANT WITH COENZYME A.  
Authors : Merilainen, G.; Poikela, V.; Kursula, P.; Wierenga, R.K.  
Deposited on : 2009-06-22  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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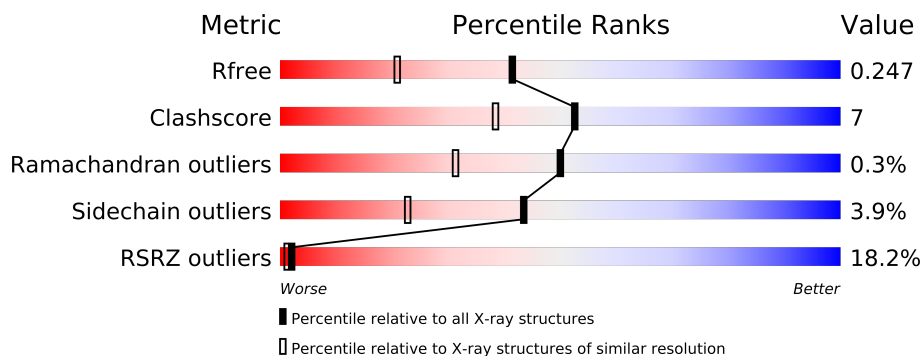
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	392	
1	B	392	
2	C	392	
2	D	392	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	1395	-	X
3	SO4	A	1397	-	X
3	SO4	B	1396	-	X
3	SO4	B	1397	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	DNO	A	1398	-	X
4	DNO	C	1397	-	X
6	NA	B	1398	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12780 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	8	0
			2856	1783	513	539	21			
1	B	389	Total	C	N	O	S	0	7	0
			2850	1775	511	541	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
A	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097

- Molecule 2 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	389	Total	C	N	O	S	0	1	0
			2815	1748	508	538	21			
2	D	389	Total	C	N	O	S	0	0	0
			2811	1744	508	538	21			

There are 4 discrepancies between the modelled and reference sequences:

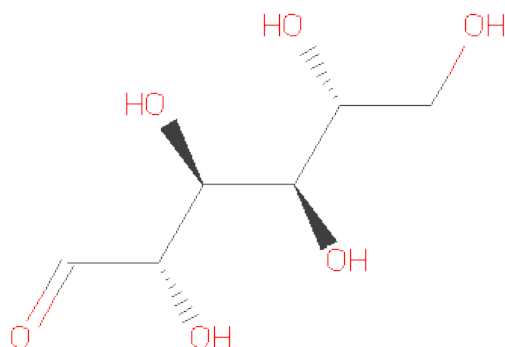
Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097
D	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



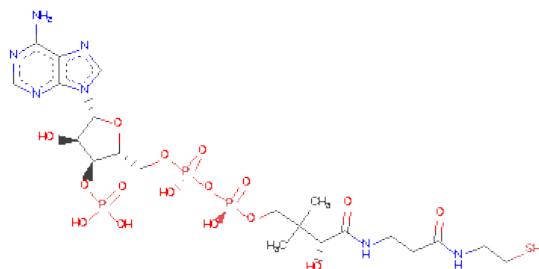
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SUGAR (D-MANNOSE) (three-letter code: DNO) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na		
			1	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl		
			1	1	0	0

- Molecule 8 is water.

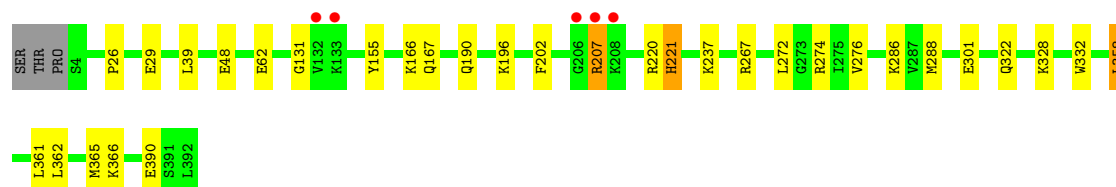
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	453	Total	O		
			453	453	0	0
8	B	479	Total	O		
			479	479	0	0
8	C	171	Total	O		
			171	171	0	0
8	D	129	Total	O		
			129	129	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

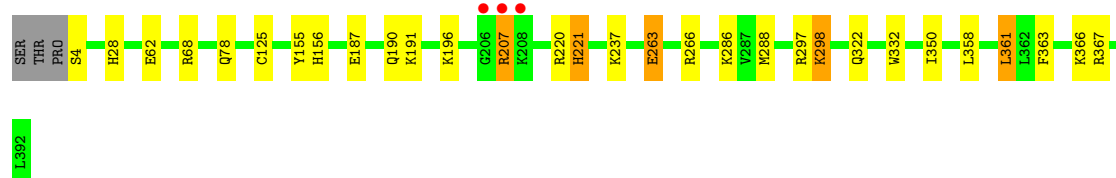
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain A: 



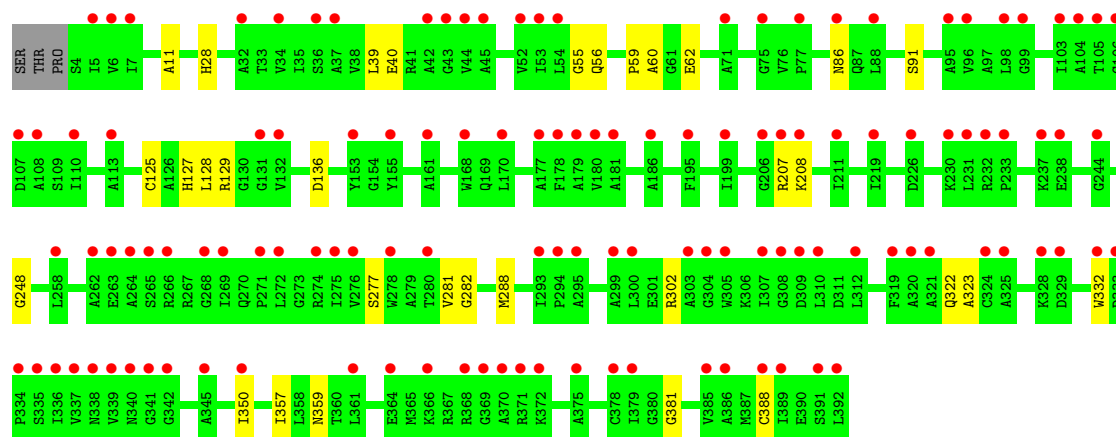
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain B: 



- Molecule 2: ACETYL-COA ACETYLTRANSFERASE

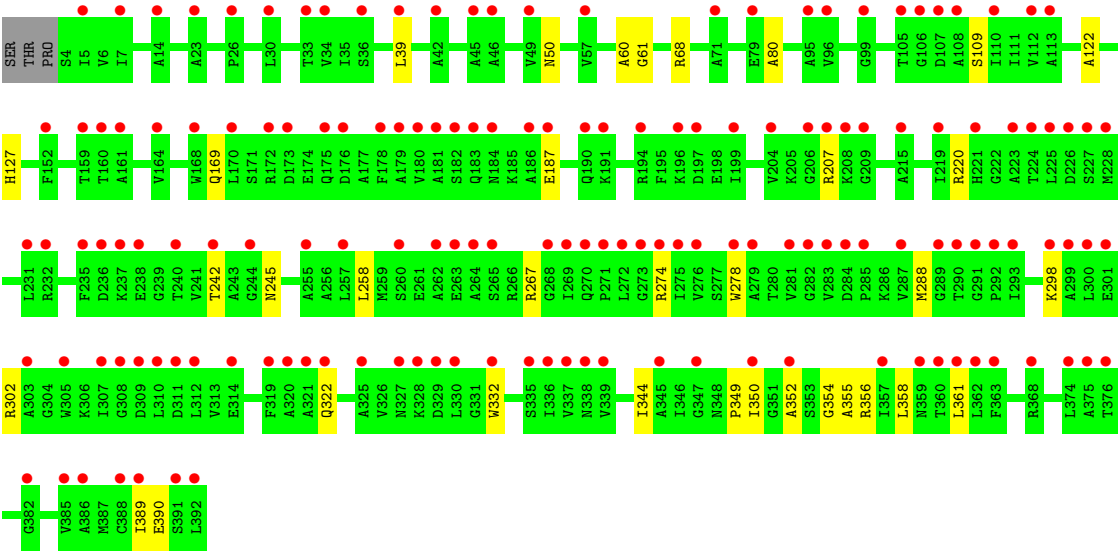
Chain C: 



- Molecule 2: ACETYL-COA ACETYLTRANSFERASE

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.70Å 79.20Å 153.00Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	19.39 – 1.80 19.39 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.39-1.80) 86.6 (19.39-1.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.221 , 0.257 0.211 , 0.247	Depositor DCC
$R_{free}$ test set	9225 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 74.0	EDS
Estimated twinning fraction	0.176 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 184510 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, CL, NA, DNO, COA, SO4

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	0.54	0/2912	0.67	0/3928
1	B	0.54	0/2900	0.69	3/3910 (0.1%)
2	C	0.27	0/2858	0.46	0/3859
2	D	0.26	0/2851	0.46	0/3849
All	All	0.43	0/11521	0.58	3/15546 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	361	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	367	ARG	NE-CZ-NH1	5.27	122.93	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2856	0	0	25	0
1	B	2850	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2815	0	0	21	0
2	D	2811	0	0	19	0
3	A	20	0	0	0	0
3	B	25	0	0	0	0
3	C	20	0	0	0	0
3	D	5	0	0	0	0
4	A	12	0	12	0	0
4	C	36	0	36	2	0
5	A	48	0	32	4	0
5	B	48	0	32	1	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	A	453	0	0	17	0
8	B	479	0	0	9	0
8	C	171	0	0	14	0
8	D	129	0	0	13	0
All	All	12780	0	112	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:125:CYS:SG	8:D:2021:HOH:O	2.30	0.89
1:B:125:CYS:SG	8:B:2183:HOH:O	2.48	0.72
2:C:136:ASP:N	4:C:1397:DNO:HO6	1.90	0.68
1:A:220[B]:ARG:NH1	8:A:2300:HOH:O	2.27	0.67
2:C:128:LEU:O	8:C:2065:HOH:O	2.14	0.65
5:A:1399:COA:H32	8:A:2198:HOH:O	1.96	0.63
2:C:381:GLY:N	8:C:2154:HOH:O	2.33	0.62
1:A:207:ARG:NH1	1:A:207:ARG:CG	2.63	0.62
1:A:202:PHE:CZ	8:A:2049:HOH:O	2.51	0.61
1:A:196[A]:LYS:NZ	8:A:2268:HOH:O	2.33	0.60
1:A:362:LEU:CD2	8:A:2344:HOH:O	2.50	0.60
1:B:263:GLU:OE1	1:B:266:ARG:NH2	2.35	0.60
1:B:297:ARG:NE	8:B:2379:HOH:O	2.34	0.59
1:A:62:GLU:CD	8:A:2085:HOH:O	2.40	0.59
5:B:1399:COA:H8A	8:B:2470:HOH:O	2.03	0.58
2:C:277:SER:N	8:C:2120:HOH:O	2.35	0.58
2:D:356:ARG:NE	8:D:2115:HOH:O	2.36	0.57
2:C:281:VAL:N	8:C:2123:HOH:O	2.38	0.56
2:D:61:GLY:CA	8:D:2021:HOH:O	2.55	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:282:GLY:CA	8:C:2155:HOH:O	2.54	0.54
1:A:301:GLU:CG	8:A:2366:HOH:O	2.55	0.54
5:A:1399:COA:O5P	5:A:1399:COA:H21	2.06	0.54
2:D:68:ARG:NH2	8:D:2026:HOH:O	2.40	0.53
1:A:220[A]:ARG:NH2	8:A:2298:HOH:O	2.41	0.53
1:A:274:ARG:NH2	1:A:390:GLU:OE1	2.42	0.52
1:A:361[A]:LEU:CD1	1:A:365:MET:SD	2.98	0.52
1:A:166:LYS:NZ	8:A:2216:HOH:O	2.42	0.51
2:D:278:TRP:O	2:D:302:ARG:NH1	2.44	0.51
2:C:388:CYS:CB	8:C:2120:HOH:O	2.59	0.51
1:B:286:LYS:NZ	8:B:2374:HOH:O	2.45	0.49
1:B:68:ARG:NH2	8:B:2114:HOH:O	2.45	0.49
2:C:127:HIS:CD2	8:D:2042:HOH:O	2.64	0.49
1:A:220[A]:ARG:NH2	8:A:2299:HOH:O	2.46	0.48
1:B:220:ARG:NH2	8:B:2309:HOH:O	2.46	0.48
2:D:68:ARG:N	8:D:2027:HOH:O	2.46	0.47
5:A:1399:COA:O7A	2:C:208:LYS:NZ	2.47	0.47
1:B:190:GLN:OE1	1:B:221:HIS:CE1	2.67	0.47
1:B:196[B]:LYS:NZ	8:B:2272:HOH:O	2.46	0.47
2:C:55:GLY:C	8:C:2029:HOH:O	2.52	0.47
1:A:167:GLN:NE2	8:A:2218:HOH:O	2.47	0.46
2:D:127:HIS:CG	8:D:2043:HOH:O	2.68	0.46
2:D:50:ASN:OD1	2:D:109:SER:N	2.48	0.46
2:C:129:ARG:NH2	2:D:122:ALA:O	2.49	0.45
1:A:286:LYS:NZ	8:A:2353:HOH:O	2.50	0.45
1:A:358[B]:LEU:CD2	1:A:362:LEU:CD1	2.94	0.45
1:A:196[B]:LYS:NZ	8:A:2266:HOH:O	2.50	0.44
2:C:11:ALA:N	2:C:359:ASN:OD1	2.50	0.44
2:C:91:SER:CB	8:C:2029:HOH:O	2.66	0.44
2:D:349:PRO:O	2:D:352:ALA:N	2.51	0.44
2:D:68:ARG:NH1	2:D:80:ALA:O	2.51	0.44
1:B:363:PHE:CD1	1:B:366[A]:LYS:NZ	2.86	0.43
2:D:389:ILE:CG2	8:D:2095:HOH:O	2.66	0.43
2:D:344:ILE:CG2	8:D:2078:HOH:O	2.66	0.43
2:D:354:GLY:N	8:D:2112:HOH:O	2.50	0.43
1:A:220[A]:ARG:CZ	5:A:1399:COA:N6A	2.81	0.43
1:B:28:HIS:ND1	1:B:62:GLU:OE2	2.51	0.43
2:C:56:GLN:N	8:C:2029:HOH:O	2.52	0.43
2:C:248:GLY:N	8:C:2141:HOH:O	2.51	0.43
1:A:48:GLU:OE1	1:A:267:ARG:NH2	2.52	0.42
2:C:28:HIS:ND1	2:C:62:GLU:OE2	2.52	0.42
1:A:207:ARG:N	1:A:207:ARG:CD	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:355:ALA:O	2:D:356:ARG:C	2.58	0.42
2:D:242:THR:N	2:D:245:ASN:OD1	2.52	0.42
2:D:60:ALA:C	8:D:2021:HOH:O	2.58	0.42
1:B:156:HIS:CD2	4:C:1397:DNO:O2	2.73	0.42
1:B:263:GLU:CD	8:B:2348:HOH:O	2.58	0.42
2:D:274:ARG:N	8:D:2095:HOH:O	2.53	0.42
2:D:274:ARG:N	2:D:390:GLU:O	2.53	0.41
2:C:323:ALA:CB	8:C:2138:HOH:O	2.67	0.41
1:A:131:GLY:CA	8:C:2065:HOH:O	2.68	0.41
1:A:29:GLU:OE1	8:A:2049:HOH:O	2.22	0.41
1:A:366:LYS:NZ	8:A:2418:HOH:O	2.52	0.41
2:D:267:ARG:NH2	8:D:2088:HOH:O	2.52	0.41
1:B:207:ARG:CG	1:B:207:ARG:NH1	2.81	0.41
1:B:187:GLU:OE2	1:B:191:LYS:NZ	2.53	0.41
1:A:26:PRO:CB	8:A:2085:HOH:O	2.68	0.41
2:C:59:PRO:O	2:C:60:ALA:C	2.59	0.41
1:A:48:GLU:OE1	1:A:267:ARG:NH1	2.54	0.41
2:C:302:ARG:CZ	8:C:2132:HOH:O	2.69	0.41
2:C:86:ASN:CB	8:C:2031:HOH:O	2.69	0.41
1:B:298:LYS:CE	8:B:2380:HOH:O	2.69	0.41
1:A:190:GLN:OE1	1:A:221:HIS:CE1	2.74	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	394/392 (100%)	378 (96%)	16 (4%)	0	100	100
1	B	393/392 (100%)	380 (97%)	12 (3%)	1 (0%)	50	31
2	C	388/392 (99%)	365 (94%)	22 (6%)	1 (0%)	50	31
2	D	387/392 (99%)	359 (93%)	26 (7%)	2 (0%)	38	19
All	All	1562/1568 (100%)	1482 (95%)	76 (5%)	4 (0%)	50	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	350	ILE
2	D	350	ILE
2	D	169	GLN
1	B	350	ILE

### 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	283/278 (102%)	269 (95%)	14 (5%)	35	15
1	B	282/278 (101%)	268 (95%)	14 (5%)	34	14
2	C	277/279 (99%)	270 (98%)	7 (2%)	60	42
2	D	276/279 (99%)	265 (96%)	11 (4%)	42	22
All	All	1118/1114 (100%)	1072 (96%)	46 (4%)	43	21

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	155	TYR
1	A	207	ARG
1	A	221	HIS
1	A	237	LYS
1	A	272[A]	LEU
1	A	272[B]	LEU
1	A	276	VAL
1	A	288	MET
1	A	322	GLN
1	A	328	LYS
1	A	332	TRP
1	A	358[A]	LEU
1	A	358[B]	LEU
1	B	4	SER
1	B	78	GLN
1	B	155	TYR

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Mol	Chain	Res	Type
1	B	207	ARG
1	B	221	HIS
1	B	237	LYS
1	B	263	GLU
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	358[A]	LEU
1	B	358[B]	LEU
1	B	361	LEU
2	C	39	LEU
2	C	40	GLU
2	C	207	ARG
2	C	288	MET
2	C	322	GLN
2	C	332	TRP
2	C	357	ILE
2	D	39	LEU
2	D	187	GLU
2	D	207	ARG
2	D	220	ARG
2	D	258	LEU
2	D	288	MET
2	D	298	LYS
2	D	322	GLN
2	D	332	TRP
2	D	358	LEU
2	D	361	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	CSO	A	89	1	6,6,7	7.62	2 (33%)	3,6,8	1.82	1 (33%)
1	CSO	B	89	1	6,6,7	7.28	3 (50%)	3,6,8	0.92	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
1	CSO	A	89	1	-	0/2/5/7	0/0/0/0
1	CSO	B	89	1	-	0/2/5/7	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	CSO	O-C	18.18	1.23	1.11
1	B	89	CSO	O-C	17.21	1.23	1.11
1	B	89	CSO	OD-SG	4.07	1.79	1.62
1	A	89	CSO	OD-SG	3.95	1.79	1.62
1	B	89	CSO	CA-C	2.10	1.52	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	CSO	CA-CB-SG	-3.08	107.54	113.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

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	SO4	A	1394	-	4,4,4	0.18	0	6,6,6	0.07	0
3	SO4	A	1395	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	A	1396	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	A	1397	-	4,4,4	0.21	0	6,6,6	0.06	0
4	DNO	A	1398	-	11,11,11	1.95	3 (27%)	14,14,14	2.04	6 (42%)
5	COA	A	1399	-	50,50,50	2.42	17 (34%)	75,75,75	2.18	16 (21%)
3	SO4	B	1394	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	B	1395	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	B	1396	-	4,4,4	0.19	0	6,6,6	0.06	0
3	SO4	B	1397	-	4,4,4	0.24	0	6,6,6	0.08	0
5	COA	B	1399	-	50,50,50	2.42	15 (30%)	75,75,75	2.31	16 (21%)
3	SO4	B	1401	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	C	1393	-	4,4,4	0.20	0	6,6,6	0.06	0
3	SO4	C	1394	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	C	1395	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	C	1396	-	4,4,4	0.21	0	6,6,6	0.09	0
4	DNO	C	1397	-	11,11,11	1.81	2 (18%)	14,14,14	1.74	5 (35%)
4	DNO	C	1398	-	11,11,11	1.88	2 (18%)	14,14,14	1.99	7 (50%)
4	DNO	C	1399	-	11,11,11	1.94	3 (27%)	14,14,14	2.02	7 (50%)
3	SO4	D	1393	-	4,4,4	0.18	0	6,6,6	0.13	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
3	SO4	A	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1397	-	-	0/0/0/0	0/0/0/0
4	DNO	A	1398	-	2/2/4/5	0/15/16/16	0/0/0/0
5	COA	A	1399	-	-	0/48/64/64	0/1/3/3
3	SO4	B	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1396	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1397	-	-	0/0/0/0	0/0/0/0
5	COA	B	1399	-	-	0/48/64/64	0/1/3/3
3	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1393	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1396	-	-	0/0/0/0	0/0/0/0
4	DNO	C	1397	-	2/2/4/5	1/15/16/16	0/0/0/0
4	DNO	C	1398	-	2/2/4/5	0/15/16/16	0/0/0/0
4	DNO	C	1399	-	2/2/4/5	0/15/16/16	0/0/0/0
3	SO4	D	1393	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1399	COA	C9P-N8P	6.70	1.48	1.33
5	A	1399	COA	C9P-N8P	6.57	1.47	1.33
5	B	1399	COA	C5P-N4P	5.75	1.46	1.33
5	A	1399	COA	C5P-N4P	5.72	1.46	1.33
5	B	1399	COA	C4A-N9A	4.86	1.44	1.37
4	A	1398	DNO	C4-C3	4.58	1.63	1.53
5	A	1399	COA	C4A-N9A	4.52	1.44	1.37
4	C	1399	DNO	C4-C3	4.51	1.62	1.53
5	B	1399	COA	P3B-O7A	4.37	1.65	1.51
4	C	1398	DNO	C4-C3	4.32	1.62	1.53
5	A	1399	COA	P1A-O3A	4.28	1.67	1.59
5	A	1399	COA	P3B-O7A	4.27	1.65	1.51
5	A	1399	COA	P2A-O3A	4.13	1.67	1.59
5	B	1399	COA	P1A-O3A	4.03	1.67	1.59
4	C	1397	DNO	C4-C3	3.96	1.61	1.53
5	A	1399	COA	C2A-N3A	3.95	1.40	1.32
5	B	1399	COA	C8A-N7A	3.87	1.42	1.34
5	B	1399	COA	C2A-N3A	3.82	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1399	COA	P1A-O1A	3.78	1.65	1.51
5	A	1399	COA	P2A-O4A	3.75	1.65	1.51
5	A	1399	COA	P1A-O1A	3.75	1.65	1.51
5	A	1399	COA	C8A-N7A	3.71	1.41	1.34
4	C	1397	DNO	O1-C1	3.71	1.38	1.19
5	B	1399	COA	P2A-O4A	3.69	1.65	1.51
4	C	1398	DNO	O1-C1	3.65	1.38	1.19
4	C	1399	DNO	O1-C1	3.62	1.38	1.19
4	A	1398	DNO	O1-C1	3.61	1.37	1.19
5	B	1399	COA	P2A-O3A	3.52	1.66	1.59
5	B	1399	COA	O4B-C1B	3.34	1.46	1.41
5	A	1399	COA	O4B-C1B	3.21	1.46	1.41
5	A	1399	COA	C6A-N6A	3.17	1.45	1.35
5	B	1399	COA	C6A-N6A	3.14	1.45	1.35
5	B	1399	COA	C2B-C1B	-2.89	1.49	1.53
5	B	1399	COA	P3B-O8A	2.89	1.65	1.54
5	A	1399	COA	P3B-O8A	2.85	1.65	1.54
5	A	1399	COA	C5A-C4A	-2.60	1.34	1.40
5	B	1399	COA	C5A-C4A	-2.47	1.34	1.40
5	A	1399	COA	C4A-N3A	-2.47	1.31	1.35
5	A	1399	COA	C8A-N9A	-2.30	1.33	1.36
5	A	1399	COA	C2B-C1B	-2.26	1.50	1.53
4	A	1398	DNO	C3-C2	2.18	1.56	1.53
4	C	1399	DNO	C3-C2	2.15	1.56	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1399	COA	N3A-C2A-N1A	-11.52	119.08	128.71
5	A	1399	COA	N3A-C2A-N1A	-10.59	119.86	128.71
5	B	1399	COA	O4B-C1B-N9A	7.57	115.48	108.44
5	A	1399	COA	C2B-C1B-N9A	6.33	129.51	113.27
5	B	1399	COA	P2A-O3A-P1A	-6.23	113.42	131.68
5	A	1399	COA	P2A-O3A-P1A	-4.90	117.33	131.68
5	B	1399	COA	C2B-C1B-N9A	4.79	125.56	113.27
5	A	1399	COA	O4B-C1B-N9A	3.97	112.13	108.44
5	B	1399	COA	N3A-C4A-N9A	3.93	132.54	125.43
5	A	1399	COA	O2B-C2B-C3B	3.79	122.34	111.20
5	A	1399	COA	N3A-C4A-N9A	3.68	132.08	125.43
5	A	1399	COA	O6A-CCP-CBP	3.67	116.70	110.57
5	A	1399	COA	C3P-N4P-C5P	-3.66	115.38	122.84
5	A	1399	COA	CBP-CAP-C9P	-3.62	109.22	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1399	COA	O2B-C2B-C1B	3.56	122.00	111.23
5	B	1399	COA	C8A-N9A-C4A	3.48	109.56	106.90
4	A	1398	DNO	O6-C6-C5	3.35	118.55	111.05
5	B	1399	COA	O3B-C3B-C4B	3.34	123.09	110.06
4	C	1399	DNO	O6-C6-C5	3.13	118.07	111.05
5	B	1399	COA	CCP-CBP-CAP	-3.09	104.19	108.70
5	B	1399	COA	O2B-C2B-C3B	3.07	120.22	111.20
5	B	1399	COA	O2B-C2B-C1B	3.03	120.40	111.23
4	C	1398	DNO	O1-C1-C2	-2.96	116.60	125.31
5	A	1399	COA	C8A-N9A-C4A	2.90	109.11	106.90
4	C	1399	DNO	O4-C4-C3	2.86	116.33	109.42
4	A	1398	DNO	C3-C2-C1	2.86	115.42	111.69
4	C	1397	DNO	O1-C1-C2	-2.85	116.94	125.31
4	C	1397	DNO	O5-C5-C4	2.77	115.94	109.05
4	A	1398	DNO	O1-C1-C2	-2.68	117.44	125.31
4	C	1399	DNO	O1-C1-C2	-2.67	117.45	125.31
5	B	1399	COA	C4B-O4B-C1B	-2.67	106.85	109.75
5	A	1399	COA	O3B-C3B-C4B	2.65	120.42	110.06
4	C	1398	DNO	O6-C6-C5	2.65	116.99	111.05
5	B	1399	COA	CDP-CBP-CCP	2.62	112.53	108.76
5	A	1399	COA	N7A-C8A-N9A	-2.60	107.00	114.36
5	B	1399	COA	N7A-C8A-N9A	-2.59	107.03	114.36
5	B	1399	COA	C7P-C6P-C5P	2.59	116.67	112.25
4	C	1398	DNO	O5-C5-C4	2.52	115.33	109.05
5	A	1399	COA	C7P-C6P-C5P	2.52	116.54	112.25
4	A	1398	DNO	O5-C5-C4	2.51	115.30	109.05
4	C	1398	DNO	C3-C2-C1	2.46	114.90	111.69
4	A	1398	DNO	O4-C4-C3	2.44	115.32	109.42
5	A	1399	COA	C5A-C4A-N3A	-2.35	120.58	125.70
4	C	1399	DNO	O5-C5-C4	2.31	114.80	109.05
4	C	1397	DNO	O3-C3-C2	2.24	112.85	108.86
5	B	1399	COA	C5A-C4A-N3A	-2.23	120.84	125.70
5	A	1399	COA	O3B-C3B-C2B	2.22	120.24	111.54
4	C	1398	DNO	O3-C3-C2	2.21	112.80	108.86
4	C	1399	DNO	O5-C5-C6	2.20	114.32	109.20
4	C	1397	DNO	O6-C6-C5	2.20	115.97	111.05
4	A	1398	DNO	O2-C2-C3	2.18	114.21	109.70
4	C	1397	DNO	O5-C5-C6	2.16	114.22	109.20
4	C	1398	DNO	O4-C4-C3	2.15	114.61	109.42
4	C	1399	DNO	O3-C3-C2	2.15	112.69	108.86
4	C	1398	DNO	O2-C2-C3	2.15	114.14	109.70
5	B	1399	COA	C2A-N3A-C4A	2.11	120.03	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	C	1399	DNO	O2-C2-C3	2.11	114.06	109.70

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1399	DNO	C2
4	C	1399	DNO	C3
4	A	1398	DNO	C2
4	A	1398	DNO	C3
4	C	1398	DNO	C2
4	C	1398	DNO	C3
4	C	1397	DNO	C2
4	C	1397	DNO	C3

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1397	DNO	O1-C1-C2-C3

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	389/392 (99%)	-0.13	5 (1%) 74 70	5, 13, 34, 96	0
1	B	389/392 (99%)	-0.17	3 (0%) 83 81	5, 13, 32, 88	0
2	C	389/392 (99%)	1.64	124 (31%) 1 1	18, 50, 79, 108	0
2	D	389/392 (99%)	1.98	154 (39%) 1 1	20, 57, 102, 131	0
All	All	1556/1568 (99%)	0.83	286 (18%) 2 1	5, 34, 81, 131	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	285	PRO	9.5
2	D	269	ILE	8.4
2	D	265	SER	8.2
2	D	207	ARG	8.2
2	D	307	ILE	8.1
2	D	227	SER	7.7
2	D	231	LEU	7.3
2	D	391	SER	7.1
2	D	308	GLY	6.6
2	D	289	GLY	6.6
2	C	303	ALA	6.5
2	C	274	ARG	6.4
2	C	299	ALA	6.4
2	C	269	ILE	6.2
2	D	108	ALA	6.2
2	C	309	ASP	6.2
2	D	5	ILE	6.1
2	C	308	GLY	6.1
2	C	110	ILE	6.0
2	C	337	VAL	6.0
2	D	325	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
2	C	391	SER	5.9
2	D	332	TRP	5.9
2	C	103	ILE	5.9
2	D	238	GLU	5.8
2	D	385	VAL	5.8
2	C	206	GLY	5.8
2	D	224	THR	5.8
2	D	270	GLN	5.7
2	C	389	ILE	5.7
2	C	386	ALA	5.6
2	D	226	ASP	5.5
2	C	375	ALA	5.4
2	D	310	LEU	5.4
2	D	335	SER	5.3
1	A	132	VAL	5.3
2	C	34[A]	VAL	5.3
2	D	368	ARG	5.2
2	D	305	TRP	5.1
2	D	279	ALA	5.1
2	D	392	LEU	5.0
2	C	264	ALA	5.0
2	C	295	ALA	5.0
2	C	276	VAL	4.9
2	C	369	GLY	4.9
1	A	207	ARG	4.8
2	C	324	CYS	4.8
2	D	225	LEU	4.8
2	C	370	ALA	4.7
2	D	228	MET	4.7
2	D	179	ALA	4.6
2	C	179	ALA	4.5
2	D	287	VAL	4.5
2	C	170	LEU	4.5
2	C	335	SER	4.5
2	D	57	VAL	4.4
2	D	303	ALA	4.4
2	C	107	ASP	4.4
2	D	389	ILE	4.4
2	C	108	ALA	4.4
2	C	262	ALA	4.4
2	C	293	ILE	4.4
2	C	238	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	209	GLY	4.3
2	D	34	VAL	4.3
2	D	95	ALA	4.3
2	D	186	ALA	4.3
2	C	340	ASN	4.3
2	D	164	VAL	4.2
2	D	173	ASP	4.2
2	D	388	CYS	4.2
2	C	186	ALA	4.1
2	D	328	LYS	4.0
2	D	293	ILE	4.0
2	D	181	ALA	4.0
2	C	52	VAL	3.9
2	D	96	VAL	3.9
2	C	177	ALA	3.9
2	D	359	ASN	3.9
2	D	178	PHE	3.9
2	D	281	VAL	3.9
2	D	161	ALA	3.9
2	D	273	GLY	3.8
2	C	266	ARG	3.8
2	D	262	ALA	3.8
2	C	106	GLY	3.8
2	D	106	GLY	3.8
2	C	321	ALA	3.8
2	D	168	TRP	3.8
2	C	392	LEU	3.8
2	D	327	ASN	3.8
2	C	278	TRP	3.7
2	C	341	GLY	3.7
2	D	107	ASP	3.7
2	D	219	ILE	3.7
2	C	334	PRO	3.6
2	D	350	ILE	3.6
2	D	352	ALA	3.6
2	D	278	TRP	3.6
2	C	304	GLY	3.6
2	C	96	VAL	3.6
2	D	199	ILE	3.5
2	D	46	ALA	3.5
2	D	320	ALA	3.5
2	D	232	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	244	GLY	3.5
2	D	301	GLU	3.5
2	D	221	HIS	3.5
2	C	366	LYS	3.4
2	D	329	ASP	3.4
2	C	219	ILE	3.4
1	B	207	ARG	3.4
2	D	337	VAL	3.4
2	C	98	LEU	3.4
2	D	255	ALA	3.3
2	D	319	PHE	3.3
2	C	275	ILE	3.3
2	D	309	ASP	3.3
2	D	175	GLN	3.3
2	C	104	ALA	3.2
2	C	105	THR	3.2
2	C	6	VAL	3.2
2	D	272	LEU	3.2
2	D	49	VAL	3.2
2	D	376	THR	3.2
2	D	42	ALA	3.2
2	C	77	PRO	3.2
2	C	231	LEU	3.1
2	D	206	GLY	3.1
2	C	237	LYS	3.1
2	C	45	ALA	3.1
2	D	257	LEU	3.1
2	D	312	LEU	3.1
2	C	95	ALA	3.1
2	D	321	ALA	3.1
2	C	36	SER	3.1
2	C	350	ILE	3.1
2	C	99	GLY	3.1
2	D	314	GLU	3.1
2	D	260	SER	3.0
2	C	368	ARG	3.0
2	C	258	LEU	3.0
1	B	208	LYS	2.9
2	C	332	TRP	2.9
2	C	385	VAL	2.9
2	D	300	LEU	2.9
2	C	307	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	264	ALA	2.9
2	C	75	GLY	2.9
2	C	226	ASP	2.9
2	D	339	VAL	2.9
2	D	36	SER	2.9
2	D	176	ASP	2.9
2	D	223	ALA	2.9
2	D	208	LYS	2.9
2	C	5	ILE	2.8
2	C	265	SER	2.8
2	D	180	VAL	2.8
2	D	99	GLY	2.8
2	D	382	GLY	2.8
2	D	276	VAL	2.8
2	D	282	GLY	2.8
2	D	360	THR	2.8
2	D	110	ILE	2.8
2	D	152	PHE	2.8
2	D	275	ILE	2.8
2	D	105	THR	2.7
2	C	161	ALA	2.7
2	D	338	ASN	2.7
2	D	71	ALA	2.7
2	D	30	LEU	2.7
2	D	159	THR	2.7
2	C	230	LYS	2.7
2	D	268	GLY	2.7
2	D	291	GLY	2.7
2	D	299	ALA	2.6
2	C	208	LYS	2.6
2	D	375	ALA	2.6
2	C	372	LYS	2.6
2	C	131	GLY	2.6
2	C	181	ALA	2.6
2	D	235	PHE	2.6
2	D	271	PRO	2.6
2	C	155	TYR	2.6
2	D	172	ARG	2.6
2	D	322	GLN	2.6
2	C	86	ASN	2.6
2	C	325	ALA	2.6
2	D	113	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	280	THR	2.6
2	C	168	TRP	2.6
2	D	274	ARG	2.6
2	C	310	LEU	2.6
2	C	388	CYS	2.6
2	D	236	ASP	2.6
2	D	386	ALA	2.5
2	C	53	ILE	2.5
2	C	336	ILE	2.5
2	C	361	LEU	2.5
2	C	43	GLY	2.5
1	A	208	LYS	2.5
2	D	191	LYS	2.5
2	C	244	GLY	2.5
2	C	195	PHE	2.5
2	C	379	ILE	2.5
2	D	7	ILE	2.5
2	D	330	LEU	2.5
2	C	320	ALA	2.5
2	C	371	ARG	2.5
2	C	7	ILE	2.5
2	C	345	ALA	2.5
2	D	14	ALA	2.5
2	D	112	VAL	2.5
2	C	338	ASN	2.4
2	D	361	LEU	2.4
2	C	272	LEU	2.4
2	C	333	ASP	2.4
2	C	339	VAL	2.4
2	D	26	PRO	2.4
2	D	374	LEU	2.4
2	C	319	PHE	2.4
2	C	342	GLY	2.4
2	D	242	THR	2.4
2	D	196	LYS	2.4
2	D	363	PHE	2.4
2	D	357	ILE	2.4
2	C	232	ARG	2.4
2	D	160	THR	2.4
2	D	284	ASP	2.3
2	D	336	ILE	2.3
1	A	133	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	88	LEU	2.3
2	C	268	GLY	2.3
2	C	378	CYS	2.3
2	C	42	ALA	2.3
2	C	364	GLU	2.3
2	D	290	THR	2.3
2	C	329	ASP	2.3
2	D	182	SER	2.3
1	B	206	GLY	2.3
2	C	71	ALA	2.3
2	D	190	GLN	2.3
2	D	345	ALA	2.3
2	C	153	TYR	2.2
2	C	132	VAL	2.2
2	C	113	ALA	2.2
1	A	206	GLY	2.2
2	D	204	VAL	2.2
2	C	54	LEU	2.2
2	C	328	LYS	2.2
2	D	33	THR	2.2
2	D	240	THR	2.2
2	C	305	TRP	2.2
2	D	184	ASN	2.2
2	C	180	VAL	2.2
2	D	283	VAL	2.2
2	D	170	LEU	2.2
2	D	263	GLU	2.2
2	D	347	GLY	2.2
2	C	312	LEU	2.2
2	C	44	VAL	2.2
2	C	300	LEU	2.2
2	D	292	PRO	2.2
2	D	23	ALA	2.1
2	C	178	PHE	2.1
2	D	79	GLU	2.1
2	D	362	LEU	2.1
2	C	211	ILE	2.1
2	D	183	GLN	2.1
2	C	233	PRO	2.1
2	D	311	ASP	2.1
2	C	207	ARG	2.1
2	D	237	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	199	ILE	2.1
2	D	39	LEU	2.1
2	D	187	GLU	2.1
2	C	271	PRO	2.1
2	D	298	LYS	2.1
2	D	194	ARG	2.1
2	C	32	ALA	2.1
2	C	37	ALA	2.1
2	D	215	ALA	2.1
2	C	294	PRO	2.0
2	C	263	GLU	2.0
2	D	45	ALA	2.0
2	D	197	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	A	89	7/8	0.08	-0.28	7,9,23,28	0
1	CSO	B	89	7/8	0.07	-1.76	2,6,26,28	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	B	1398	1/1	1.47	189.14	123,123,123,123	0
3	SO4	B	1397	5/5	0.28	17.33	71,71,73,77	0
3	SO4	B	1396	5/5	0.31	15.25	77,80,81,82	0
4	DNO	C	1397	12/12	0.23	13.18	44,55,91,93	0
4	DNO	A	1398	12/12	0.31	10.05	42,52,75,76	0
3	SO4	A	1395	5/5	0.15	4.11	43,50,53,57	0
3	SO4	A	1397	5/5	0.15	2.62	72,73,76,77	0
3	SO4	C	1394	5/5	0.33	1.20	129,131,131,131	0
3	SO4	C	1396	5/5	0.29	0.46	64,66,67,71	0
3	SO4	C	1395	5/5	0.31	0.34	81,83,86,87	0
4	DNO	C	1398	12/12	0.31	0.27	57,65,78,79	0
3	SO4	B	1394	5/5	0.10	0.17	30,39,41,43	0
5	COA	A	1399	48/48	0.12	0.17	15,28,76,107	0
5	COA	B	1399	48/48	0.10	0.15	12,27,61,75	0
3	SO4	B	1395	5/5	0.10	-0.64	41,44,47,48	0
4	DNO	C	1399	12/12	0.23	-0.78	42,55,72,72	0
3	SO4	C	1393	5/5	0.18	-1.39	75,77,78,79	0
3	SO4	A	1394	5/5	0.08	-1.81	40,44,50,56	0
3	SO4	D	1393	5/5	0.10	-2.48	61,62,65,67	0
7	CL	B	1400	1/1	0.13	-	68,68,68,68	0
3	SO4	A	1396	5/5	0.17	-	64,64,66,66	0
3	SO4	B	1401	5/5	0.27	-	89,90,91,92	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.