



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2017 – 07:30 PM EDT

PDB ID : 1DLV
Title : BIOSYNTHETIC THIOLASE FROM ZOOGLOEA RAMIGERA IN COM-
PLEX WITH COA
Authors : Modis, Y.; Wierenga, R.K.
Deposited on : unknown
Resolution : 2.29 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

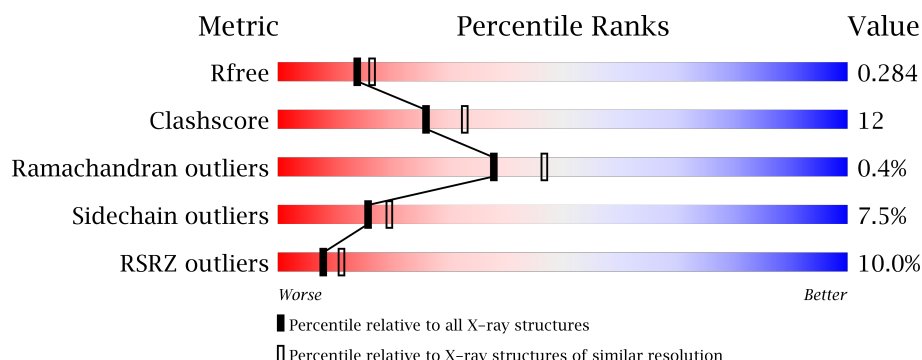
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 ≥ 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	389	<div> <div>13%</div> <div>57% 34% 8%</div> </div>
1	B	389	<div> <div>61% 30% 7%</div> </div>
1	C	389	<div> <div>25%</div> <div>70% 24% 5%</div> </div>
1	D	389	<div> <div>69% 26% 5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12192 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 BIOSYNTHETIC THIOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	B	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	C	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	D	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	INSERTION	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	11	ALA	-	INSERTION	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	11	ALA	-	INSERTION	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	11	ALA	-	INSERTION	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

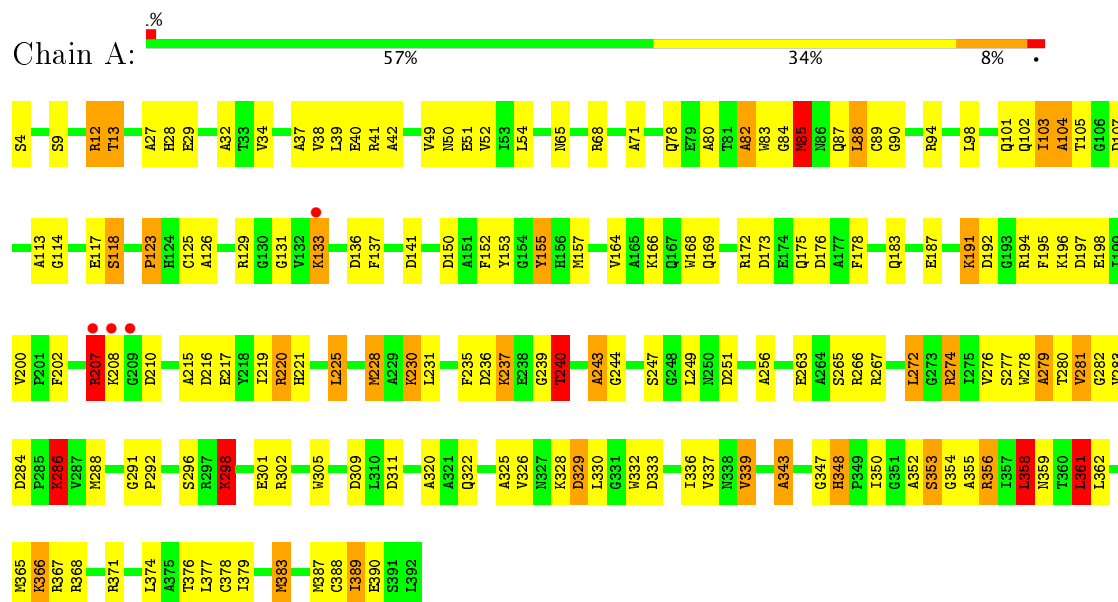
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total	O	1	0
			287	287		
4	B	276	Total	O	3	0
			276	276		
4	C	96	Total	O	0	0
			96	96		
4	D	59	Total	O	1	0
			59	59		

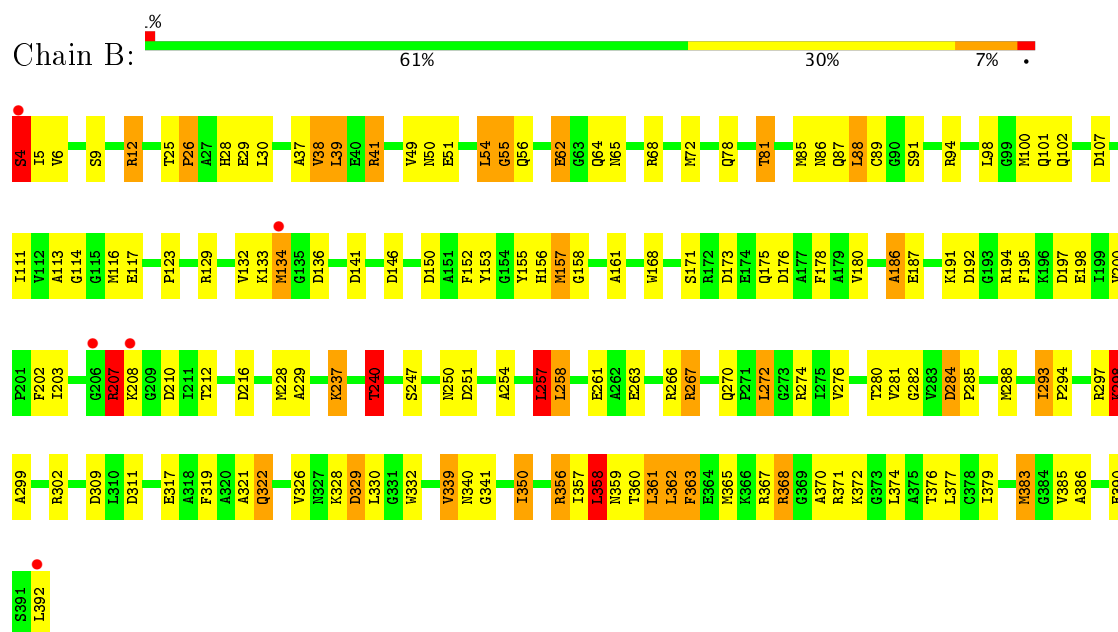
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

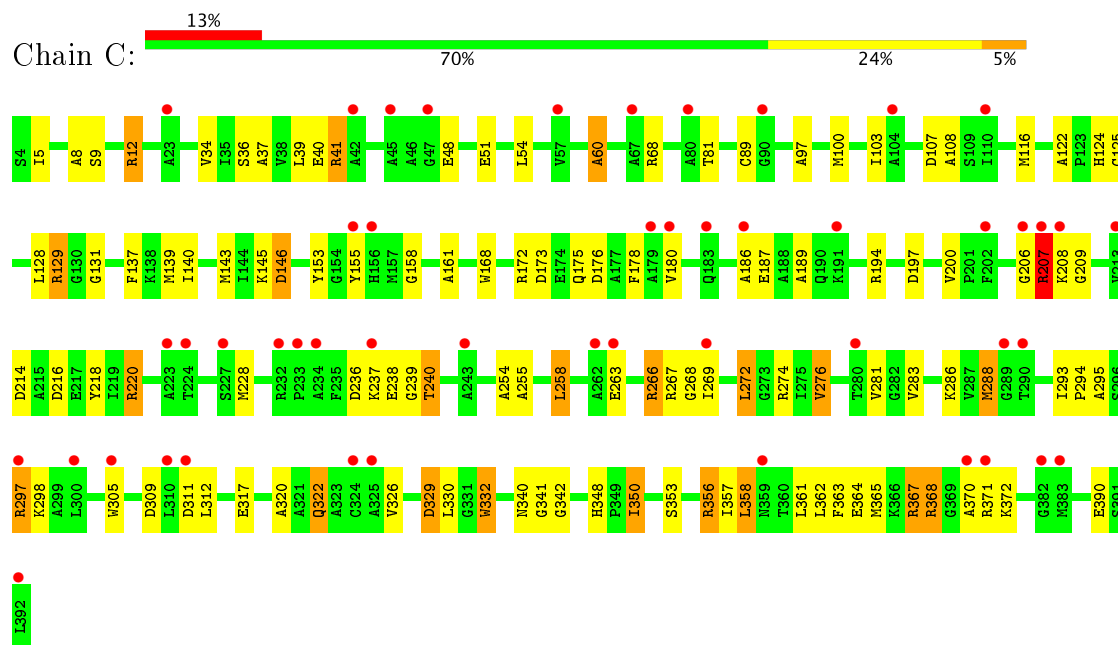
• Molecule 1: BIOSYNTHETIC THIOLASE



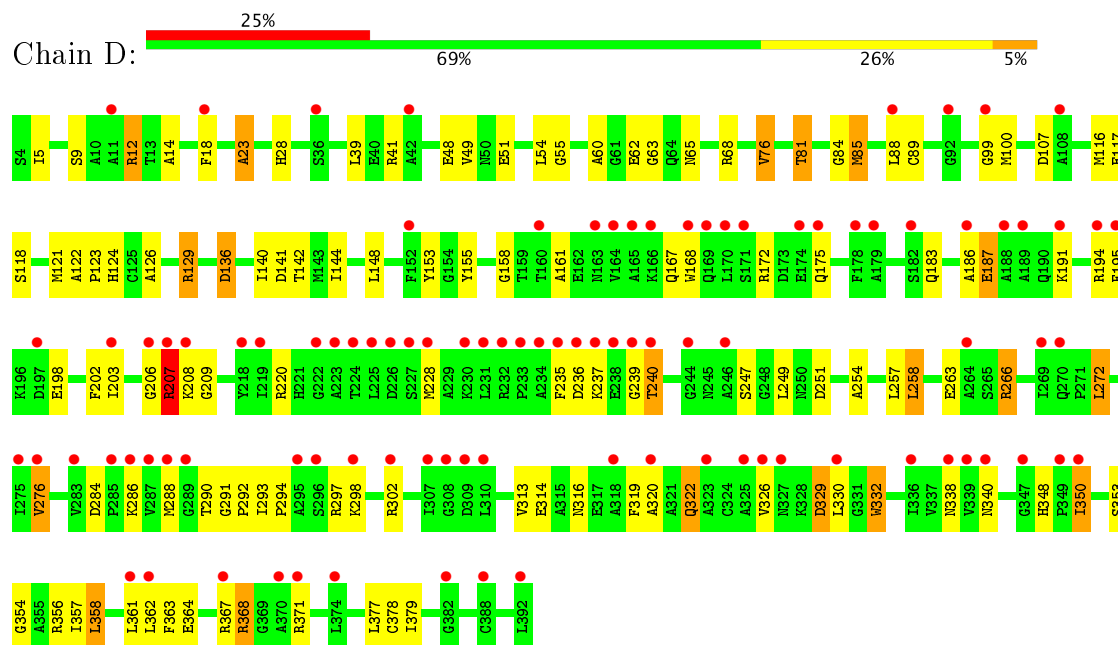
• Molecule 1: BIOSYNTHETIC THIOLASE



• Molecule 1: BIOSYNTHETIC THIOLASE



• Molecule 1: BIOSYNTHETIC THIOLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.82Å 79.30Å 149.98Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	30.00 – 2.29 29.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.29) 82.2 (29.51-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.293 0.238 , 0.284	Depositor DCC
R_{free} test set	4441 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12192	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.74% 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, 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	1.24	7/2854 (0.2%)	2.64	181/3853 (4.7%)
1	B	1.22	7/2854 (0.2%)	2.32	142/3853 (3.7%)
1	C	0.61	0/2854	1.67	46/3853 (1.2%)
1	D	0.60	0/2854	1.71	55/3853 (1.4%)
All	All	0.97	14/11416 (0.1%)	2.12	424/15412 (2.8%)

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

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	LEU	C-N	20.46	1.69	1.33
1	A	278	TRP	CZ2-CH2	-12.08	1.14	1.37
1	A	118	SER	CA-CB	11.31	1.70	1.52
1	A	278	TRP	CZ3-CH2	10.95	1.57	1.40
1	A	90	GLY	N-CA	8.92	1.59	1.46

The worst 5 of 424 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	NE-CZ-NH1	22.74	131.67	120.30
1	A	367	ARG	NE-CZ-NH1	22.35	131.47	120.30
1	A	251	ASP	CB-CG-OD1	21.21	137.39	118.30
1	C	266	ARG	NE-CZ-NH2	20.53	130.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	ASP	CB-CG-OD2	20.18	136.46	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ILE	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2813	0	2818	68	0
1	B	2813	0	2819	72	0
1	C	2813	0	2819	64	0
1	D	2813	0	2819	70	0
2	A	15	0	0	0	0
2	B	15	0	0	1	0
3	A	48	0	32	4	0
3	B	48	0	31	2	0
3	C	48	0	31	0	0
3	D	48	0	31	2	0
4	A	287	0	0	13	2
4	B	276	0	0	17	1
4	C	96	0	0	14	0
4	D	59	0	0	10	0
All	All	12192	0	11400	269	3

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 12.

The worst 5 of 269 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:B:54:LEU:C	1:B:55:GLY:N	1.69	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.25	1.00
1:B:258:LEU:HG	4:B:5222:HOH:O	1.65	0.97
1:A:175:GLN:HE22	1:A:240:THR:CG2	1.79	0.95
1:B:356:ARG:HD2	1:B:356:ARG:C	1.92	0.89

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:5238:HOH:O	4:A:5280:HOH:O[2_645]	1.94	0.26
4:A:5078:HOH:O	4:A:5084:HOH:O[2_655]	2.13	0.07
4:B:5202:HOH:O	4:B:5234:HOH:O[2_555]	2.16	0.04

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	387/389 (100%)	369 (95%)	17 (4%)	1 (0%)	44	55
1	B	387/389 (100%)	376 (97%)	10 (3%)	1 (0%)	44	55
1	C	387/389 (100%)	365 (94%)	21 (5%)	1 (0%)	44	55
1	D	387/389 (100%)	370 (96%)	14 (4%)	3 (1%)	22	26
All	All	1548/1556 (100%)	1480 (96%)	62 (4%)	6 (0%)	38	47

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	ILE
1	D	350	ILE
1	B	350	ILE
1	D	23	ALA
1	D	65	ASN

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	276/276 (100%)	250 (91%)	26 (9%)	10	12
1	B	276/276 (100%)	255 (92%)	21 (8%)	15	19
1	C	276/276 (100%)	258 (94%)	18 (6%)	20	26
1	D	276/276 (100%)	258 (94%)	18 (6%)	20	26
All	All	1104/1104 (100%)	1021 (92%)	83 (8%)	16	19

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	270	GLN
1	B	361	LEU
1	D	298	LYS
1	B	272	LEU
1	B	328	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	184	ASN
1	D	316	ASN
1	C	175	GLN
1	B	175	GLN
1	C	78	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	COA	A	1001	-	43,50,50	2.20	13 (30%)	48,75,75	3.13	22 (45%)
2	SO4	A	5002	-	4,4,4	0.72	0	6,6,6	0.34	0
2	SO4	A	5004	-	4,4,4	0.83	0	6,6,6	0.73	0
2	SO4	A	5005	-	4,4,4	0.89	0	6,6,6	0.66	0
3	COA	B	2001	-	43,50,50	1.91	12 (27%)	48,75,75	2.55	12 (25%)
2	SO4	B	5001	-	4,4,4	0.88	0	6,6,6	0.44	0
2	SO4	B	5003	-	4,4,4	0.82	0	6,6,6	0.26	0
2	SO4	B	5006	-	4,4,4	0.62	0	6,6,6	0.62	0
3	COA	C	3001	-	43,50,50	1.97	10 (23%)	48,75,75	2.02	11 (22%)
3	COA	D	4001	-	43,50,50	1.96	12 (27%)	48,75,75	2.12	12 (25%)

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	COA	A	1001	-	-	0/44/64/64	0/3/3/3
2	SO4	A	5002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	5004	-	-	0/0/0/0	0/0/0/0
2	SO4	A	5005	-	-	0/0/0/0	0/0/0/0
3	COA	B	2001	-	-	0/44/64/64	0/3/3/3
2	SO4	B	5001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	5003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	5006	-	-	0/0/0/0	0/0/0/0
3	COA	C	3001	-	-	0/44/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	D	4001	-	-	0/44/64/64	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	COA	C2B-C1B	-2.87	1.49	1.53
3	C	3001	COA	C9P-N8P	-2.65	1.28	1.33
3	B	2001	COA	C9P-N8P	-2.59	1.28	1.33
3	A	1001	COA	C5A-N7A	-2.49	1.31	1.39
3	B	2001	COA	C7P-C6P	-2.40	1.43	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	COA	C2P-C3P-N4P	-10.26	90.19	112.50
3	A	1001	COA	O6A-CCP-CBP	-6.70	99.78	110.55
3	A	1001	COA	C7P-N8P-C9P	-5.41	112.51	122.59
3	D	4001	COA	C2P-C3P-N4P	-5.22	101.14	112.50
3	B	2001	COA	C6P-C5P-N4P	-4.62	108.53	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	COA	4	0
3	B	2001	COA	2	0
2	B	5001	SO4	1	0
3	D	4001	COA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	54:LEU	C	55:GLY	N	1.69

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	389/389 (100%)	-0.21	4 (1%) 82 86	8, 17, 38, 83	0
1	B	389/389 (100%)	-0.15	5 (1%) 77 81	7, 18, 41, 95	0
1	C	389/389 (100%)	0.79	49 (12%) 4 6	16, 42, 74, 116	0
1	D	389/389 (100%)	1.29	98 (25%) 1 1	19, 48, 102, 127	0
All	All	1556/1556 (100%)	0.43	156 (10%) 8 11	7, 35, 75, 127	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	228	MET	8.0
1	D	307	ILE	7.0
1	D	330	LEU	6.7
1	D	164	VAL	6.1
1	D	169	GLN	5.9

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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	5006	5/5	0.93	0.16	1.79	39,41,43,43	0
3	COA	D	4001	48/48	0.69	0.28	0.47	79,112,123,124	0
3	COA	B	2001	48/48	0.93	0.13	-0.01	15,29,52,57	0
3	COA	A	1001	48/48	0.93	0.13	-0.09	12,29,45,47	0
3	COA	C	3001	48/48	0.80	0.20	-0.17	56,78,93,95	0
2	SO4	A	5004	5/5	0.96	0.10	-1.22	47,49,51,54	0
2	SO4	B	5001	5/5	0.90	0.14	-	56,56,58,58	0
2	SO4	A	5005	5/5	0.86	0.20	-	48,50,51,54	0
2	SO4	A	5002	5/5	0.95	0.13	-	58,60,61,62	0
2	SO4	B	5003	5/5	0.97	0.13	-	50,52,54,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.