



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:02 am GMT

PDB ID : 3Q0G
Title : Crystal Structure of the Mycobacterium tuberculosis Crotonase Bound to a Reaction Intermediate Derived from Crotonyl CoA
Authors : Bruning, J.B.; Delgado, E.; Ghosh, S.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2010-12-15
Resolution : 2.38 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 : trunk28620
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) : recalc28949

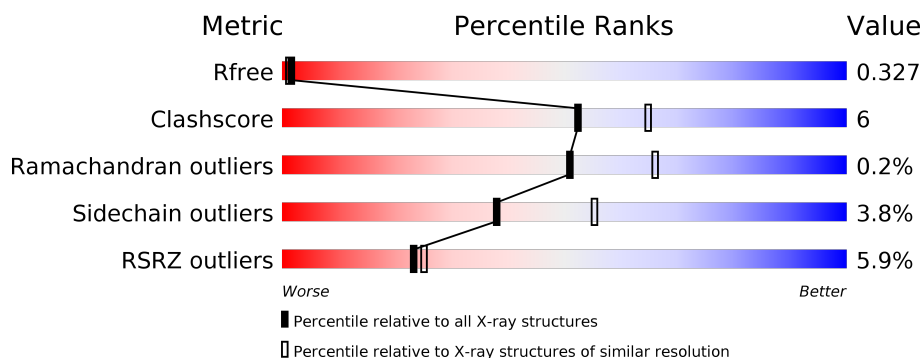
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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	257	<div> <div>5%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
1	B	257	<div> <div>5%</div> <div>82%</div> <div>16%</div> <div>•</div> </div>
1	C	257	<div> <div>7%</div> <div>86%</div> <div>13%</div> <div>• •</div> </div>
1	D	257	<div> <div>4%</div> <div>87%</div> <div>9%</div> <div>• •</div> </div>
1	E	257	<div> <div>7%</div> <div>85%</div> <div>12%</div> <div>• •</div> </div>
1	F	257	<div> <div>6%</div> <div>81%</div> <div>18%</div> <div>•</div> </div>

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
4	COA	C	258	-	-	-	X
5	BCO	F	259	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12127 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.

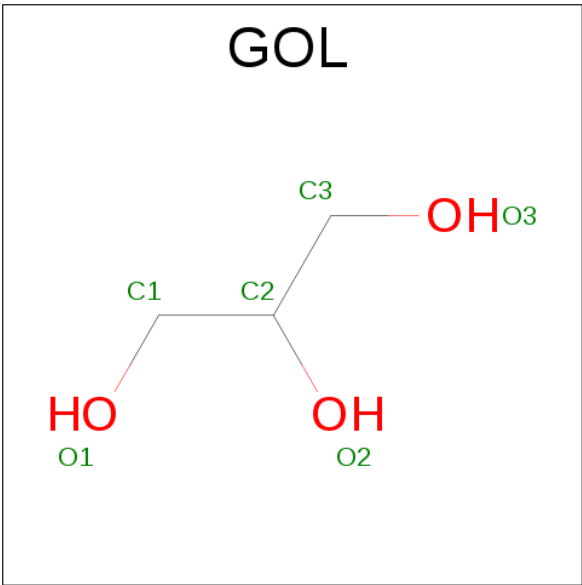
- Molecule 1 is a protein called enoyl-CoA hydratase echA8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	1	0
			1840	1147	321	361	11			
1	B	253	Total	C	N	O	S	0	0	0
			1866	1164	322	368	12			
1	C	255	Total	C	N	O	S	0	1	0
			1878	1172	324	370	12			
1	D	250	Total	C	N	O	S	0	1	0
			1831	1140	318	362	11			
1	E	253	Total	C	N	O	S	0	2	0
			1857	1158	323	364	12			
1	F	254	Total	C	N	O	S	0	3	0
			1885	1176	326	371	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

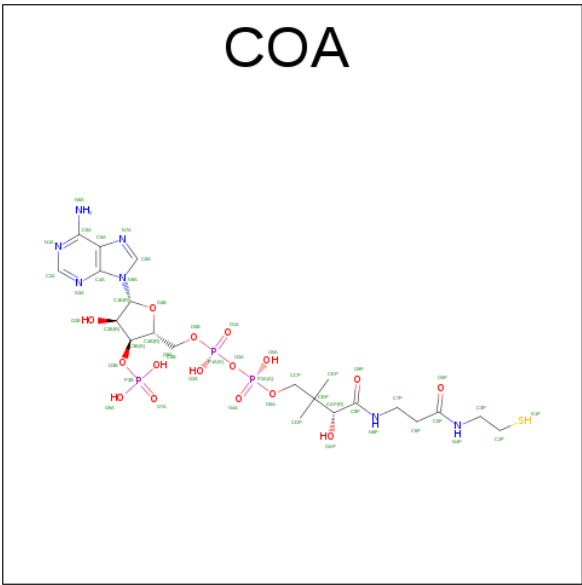
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



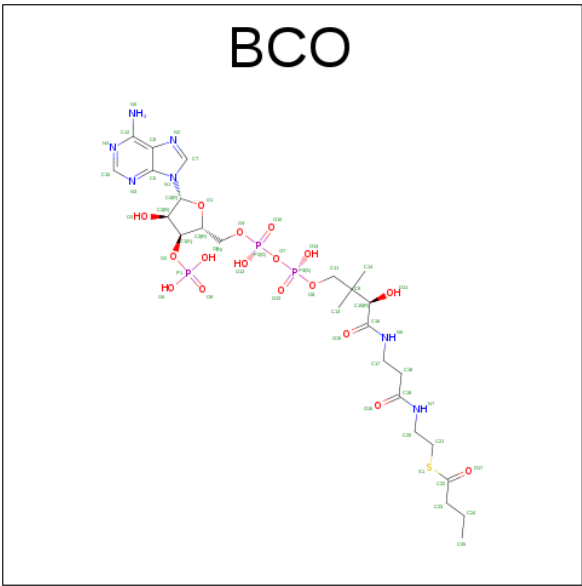
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

- Molecule 5 is BUTYRYL COENZYME A (three-letter code: BCO) (formula: C₂₅H₄₂N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	S	
			53	25	7	17	3	1	

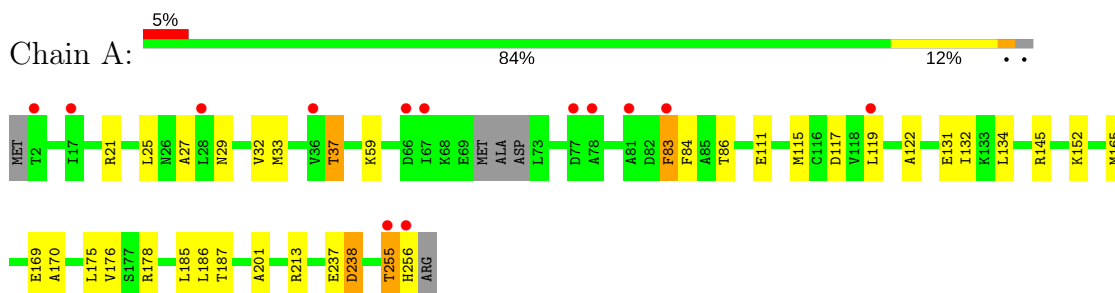
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O		
			123	123	0	0
6	B	140	Total	O		
			140	140	0	0
6	C	152	Total	O		
			152	152	0	0
6	D	141	Total	O		
			141	141	0	0
6	E	144	Total	O		
			144	144	0	0
6	F	149	Total	O		
			149	149	0	0

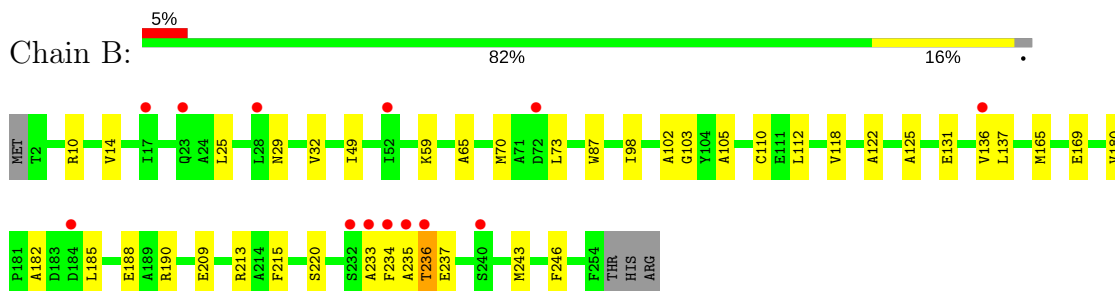
3 Residue-property plots [i](#)

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.

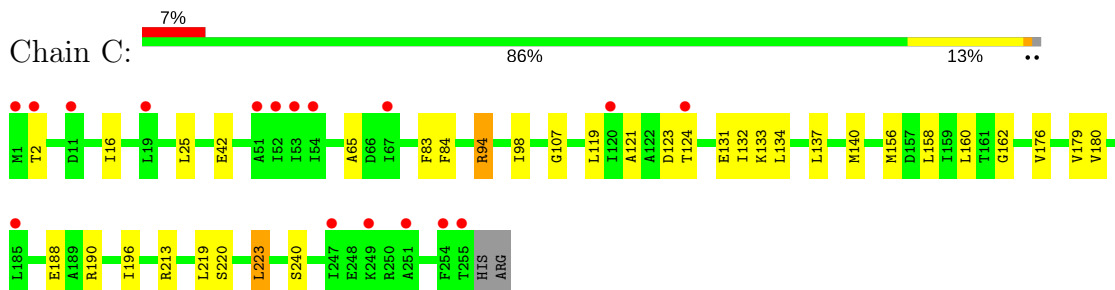
• Molecule 1: enoyl-CoA hydratase echA8



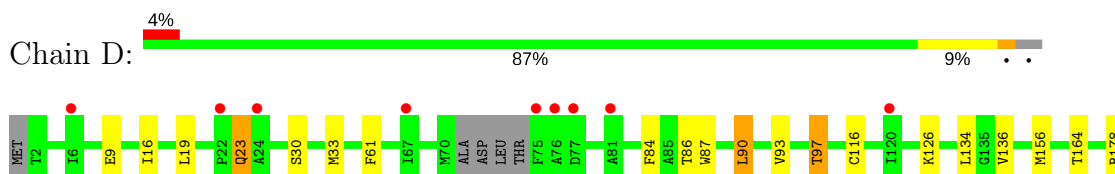
• Molecule 1: enoyl-CoA hydratase echA8



• Molecule 1: enoyl-CoA hydratase echA8

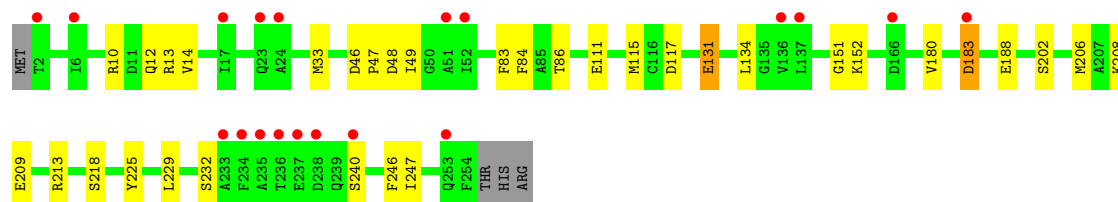
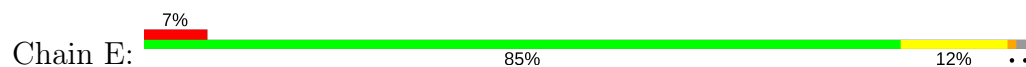


• Molecule 1: enoyl-CoA hydratase echA8

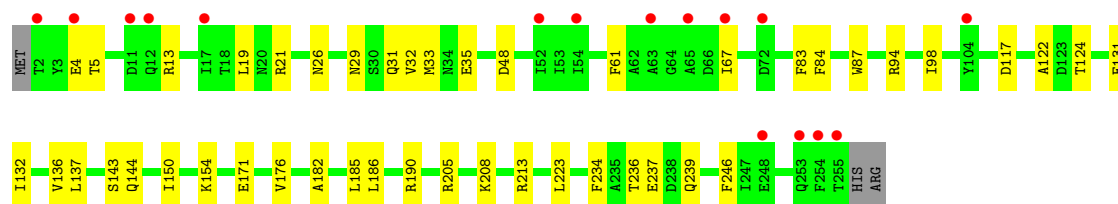
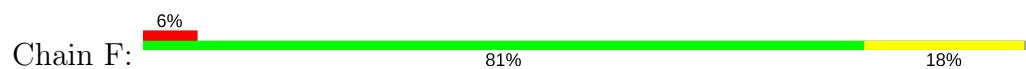




- Molecule 1: enoyl-CoA hydratase echA8



- Molecule 1: enoyl-CoA hydratase echA8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.64Å 133.17Å 133.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.38 19.87 – 2.38	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.87-2.38) 93.1 (19.87-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.233 , 0.288 0.277 , 0.327	Depositor DCC
R_{free} test set	3440 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12127	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.46 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8312e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, GOL, MG, BCO

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	0.50	0/1866	0.62	0/2524
1	B	0.48	0/1889	0.63	0/2555
1	C	0.51	0/1904	0.64	1/2576 (0.0%)
1	D	0.49	0/1856	0.61	0/2510
1	E	0.49	0/1885	0.61	0/2549
1	F	0.50	0/1917	0.63	0/2592
All	All	0.49	0/11317	0.62	1/15306 (0.0%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	THR	Peptide

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Mol	Chain	Res	Type	Group
1	B	234	PHE	Peptide

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	1840	0	1807	23	0
1	B	1866	0	1861	23	0
1	C	1878	0	1876	26	0
1	D	1831	0	1804	23	0
1	E	1857	0	1857	24	0
1	F	1885	0	1886	26	0
2	A	1	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	3	0
3	D	6	0	8	0	0
4	C	48	0	31	8	0
5	F	53	0	38	8	0
6	A	123	0	0	2	0
6	B	140	0	0	3	0
6	C	152	0	0	1	0
6	D	141	0	0	0	0
6	E	144	0	0	4	0
6	F	149	0	0	5	0
All	All	12127	0	11184	142	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 6.

The worst 5 of 142 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)
5:F:259:BCO:H35	6:F:1000:HOH:O	1.32	1.27
1:E:206:MET:HE1	6:E:502:HOH:O	1.54	1.05
1:C:156:MET:HE3	1:C:160:LEU:HD11	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ARG:HG2	1:C:94:ARG:HH11	1.28	0.95
1:C:132:ILE:O	1:C:133:LYS:HG2	1.68	0.93

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	249/257 (97%)	241 (97%)	7 (3%)	1 (0%)	38	51
1	B	251/257 (98%)	240 (96%)	10 (4%)	1 (0%)	38	51
1	C	254/257 (99%)	243 (96%)	11 (4%)	0	100	100
1	D	247/257 (96%)	240 (97%)	7 (3%)	0	100	100
1	E	253/257 (98%)	242 (96%)	10 (4%)	1 (0%)	38	51
1	F	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
All	All	1509/1542 (98%)	1452 (96%)	54 (4%)	3 (0%)	51	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	ASP
1	B	236	THR
1	E	12	GLN

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/192 (94%)	172 (96%)	8 (4%)	33	48
1	B	186/192 (97%)	181 (97%)	5 (3%)	50	68
1	C	187/192 (97%)	178 (95%)	9 (5%)	30	44
1	D	181/192 (94%)	170 (94%)	11 (6%)	22	32
1	E	185/192 (96%)	181 (98%)	4 (2%)	57	75
1	F	189/192 (98%)	184 (97%)	5 (3%)	51	70
All	All	1108/1152 (96%)	1066 (96%)	42 (4%)	38	55

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	213	ARG
1	D	30	SER
1	F	137	LEU
1	C	220	SER
1	C	240	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	31	GLN
1	F	31	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	GOL	A	401	-	5,5,5	0.35	0	5,5,5	0.38	0
3	GOL	B	402	-	5,5,5	0.33	0	5,5,5	0.63	0
4	COA	C	258	-	43,50,50	2.92	19 (44%)	48,75,75	3.93	23 (47%)
3	GOL	D	403	-	5,5,5	0.33	0	5,5,5	0.22	0
5	BCO	F	259	2	48,55,55	2.23	14 (29%)	55,81,81	3.51	24 (43%)

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	GOL	A	401	-	-	0/4/4/4	0/0/0/0
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0
4	COA	C	258	-	-	0/44/64/64	0/3/3/3
3	GOL	D	403	-	-	0/4/4/4	0/0/0/0
5	BCO	F	259	2	1/1/12/14	0/50/70/70	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	258	COA	P3B-O3B	-9.25	1.43	1.59
4	C	258	COA	P1A-O5B	-7.87	1.25	1.59
5	F	259	BCO	P2-O4	-6.80	1.30	1.59
4	C	258	COA	O4B-C4B	-5.98	1.31	1.45
5	F	259	BCO	P1-O2	-5.18	1.50	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	258	COA	N3A-C2A-N1A	-12.51	117.96	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	258	COA	C4B-O4B-C1B	-9.44	99.72	109.77
5	F	259	BCO	C10-C16-N6	-8.39	99.12	116.58
4	C	258	COA	C2B-C3B-C4B	-7.66	89.53	103.23
5	F	259	BCO	C2-C1-C3	-6.96	90.78	103.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	259	BCO	C10

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	GOL	3	0
4	C	258	COA	8	0
5	F	259	BCO	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 [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	252/257 (98%)	0.61	13 (5%) 28 30	21, 42, 74, 102	0
1	B	253/257 (98%)	0.58	13 (5%) 29 31	20, 46, 86, 141	0
1	C	255/257 (99%)	0.56	17 (6%) 19 19	22, 42, 65, 79	0
1	D	250/257 (97%)	0.51	11 (4%) 35 37	22, 42, 67, 86	0
1	E	253/257 (98%)	0.65	19 (7%) 15 16	21, 47, 74, 96	0
1	F	254/257 (98%)	0.55	16 (6%) 21 22	23, 41, 65, 82	0
All	All	1517/1542 (98%)	0.58	89 (5%) 23 25	20, 43, 72, 141	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	THR	5.1
1	B	235	ALA	5.0
1	A	256	HIS	4.7
1	D	75	PHE	4.6
1	E	2	THR	4.5

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(Å ²)	Q<0.9
4	COA	C	258	48/48	0.81	0.31	2.59	34,40,42,45	0
3	GOL	B	402	6/6	0.81	0.23	1.46	34,35,35,36	0
5	BCO	F	259	53/53	0.85	0.25	1.34	28,40,42,45	1
3	GOL	A	401	6/6	0.88	0.18	0.78	37,38,39,39	0
3	GOL	D	403	6/6	0.89	0.15	-0.52	28,31,32,32	0
2	MG	A	258	1/1	0.43	0.24	-	61,61,61,61	0
2	MG	F	258	1/1	0.42	0.21	-	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.