



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:59 PM GMT

PDB ID : 1REQ
Title : METHYLMALONYL-COA MUTASE
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1996-01-19
Resolution : 2.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

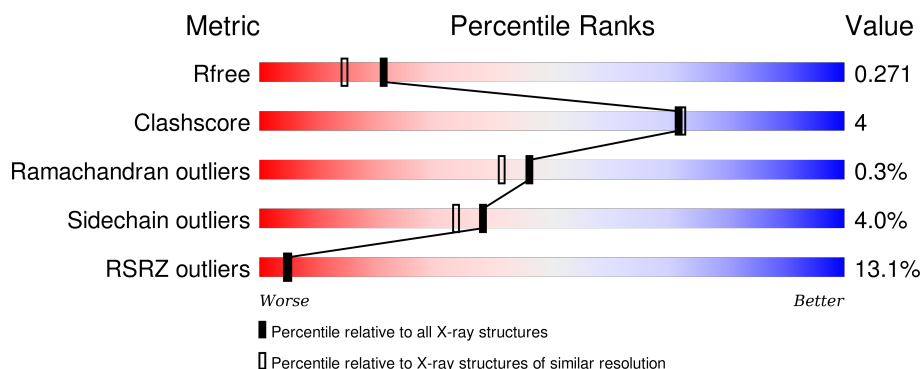
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	727	<div> <div>6%</div> <div>71%</div> <div>26%</div> <div>.</div> </div>
1	C	727	<div> <div>9%</div> <div>69%</div> <div>26%</div> <div>5%</div> <div>.</div> </div>
2	B	637	<div> <div>11%</div> <div>70%</div> <div>23%</div> <div>.</div> <div>.</div> <div>.</div> </div>
2	D	637	<div> <div>28%</div> <div>70%</div> <div>22%</div> <div>5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	1	-	-	-	X
5	GOL	B	640	-	-	-	X
5	GOL	D	639	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22372 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 METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5563	3514	960	1065	24			
1	C	727	Total	C	N	O	S	0	0	0
			5560	3515	960	1061	24			

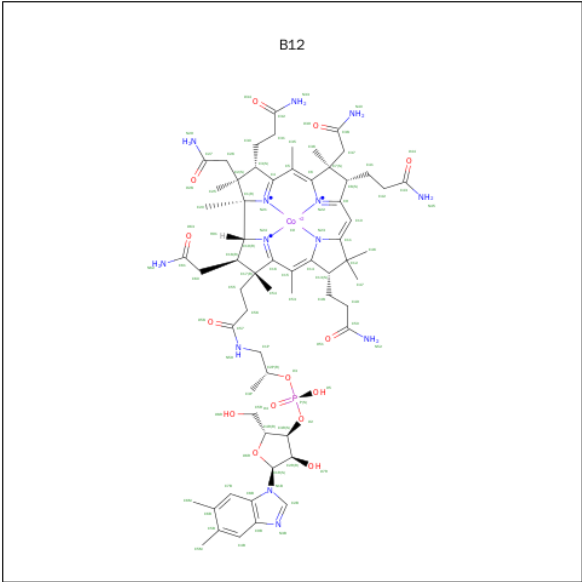
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			4695	2962	820	900	13			
2	D	622	Total	C	N	O	S	0	0	0
			4692	2958	818	903	13			

There are 6 discrepancies between the modelled and reference sequences:

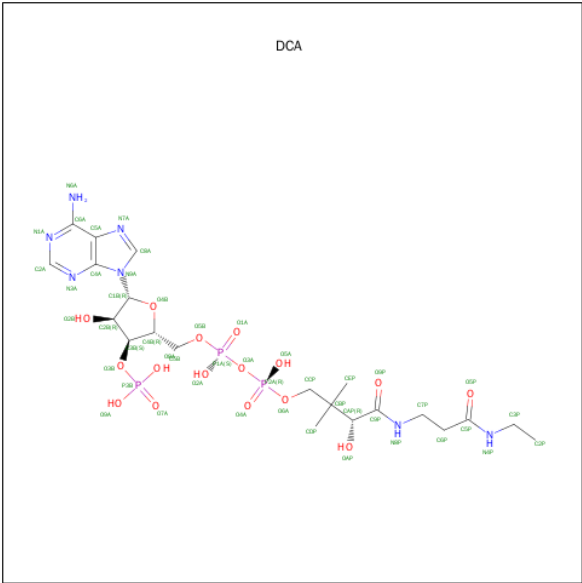
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	CONFLICT	UNP P11652
B	330	GLU	ASP	CONFLICT	UNP P11652
B	331	LEU	VAL	CONFLICT	UNP P11652
D	203	GLY	ALA	CONFLICT	UNP P11652
D	330	GLU	ASP	CONFLICT	UNP P11652
D	331	LEU	VAL	CONFLICT	UNP P11652

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is DESULFO-COENZYME A (three-letter code: DCA) (formula: C₂₁H₃₆N₇O₁₆P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			47	21	7	16	3		
4	C	1	Total	C	N	O	P	0	0
			47	21	7	16	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

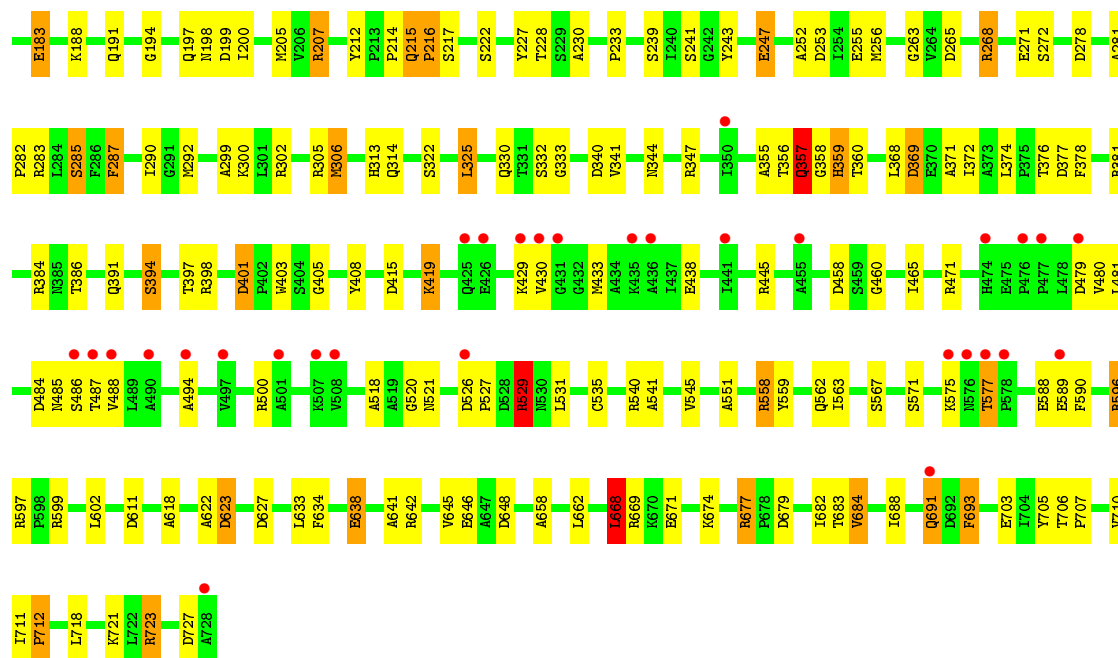
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	457	Total	O	0	0
			457	457		
6	B	318	Total	O	0	0
			318	318		

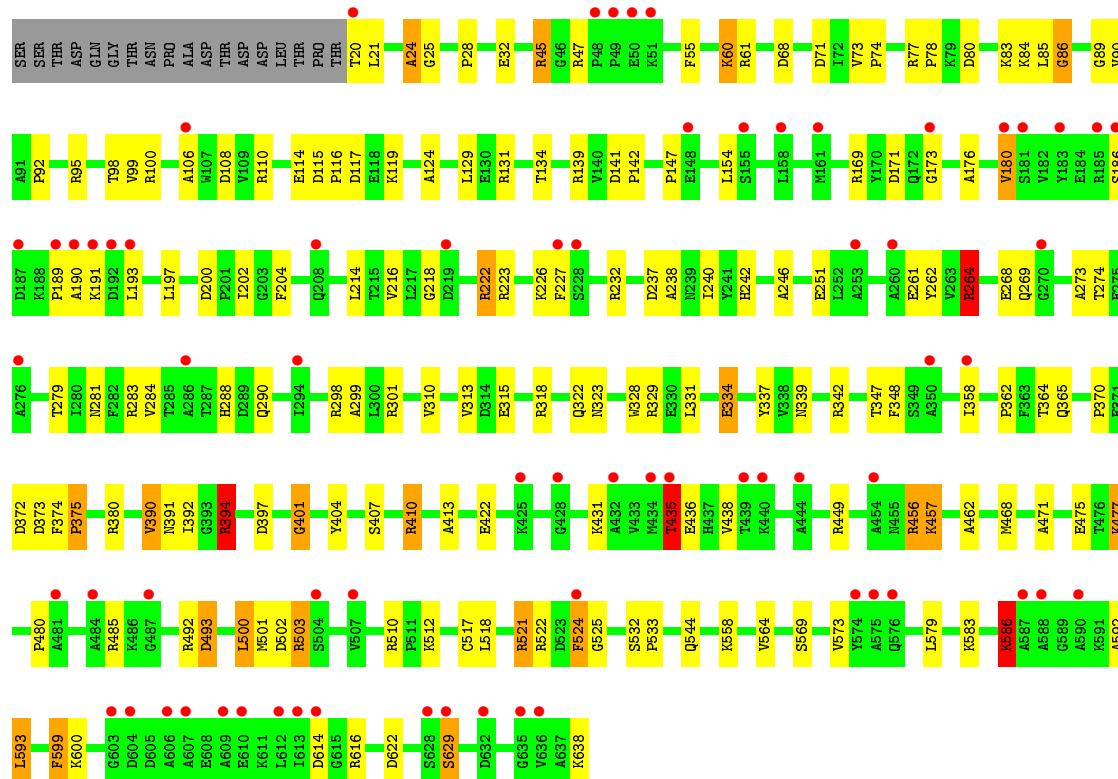
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	493	Total 493	O 493	0	0
6	D	264	Total 264	O 264	0	0

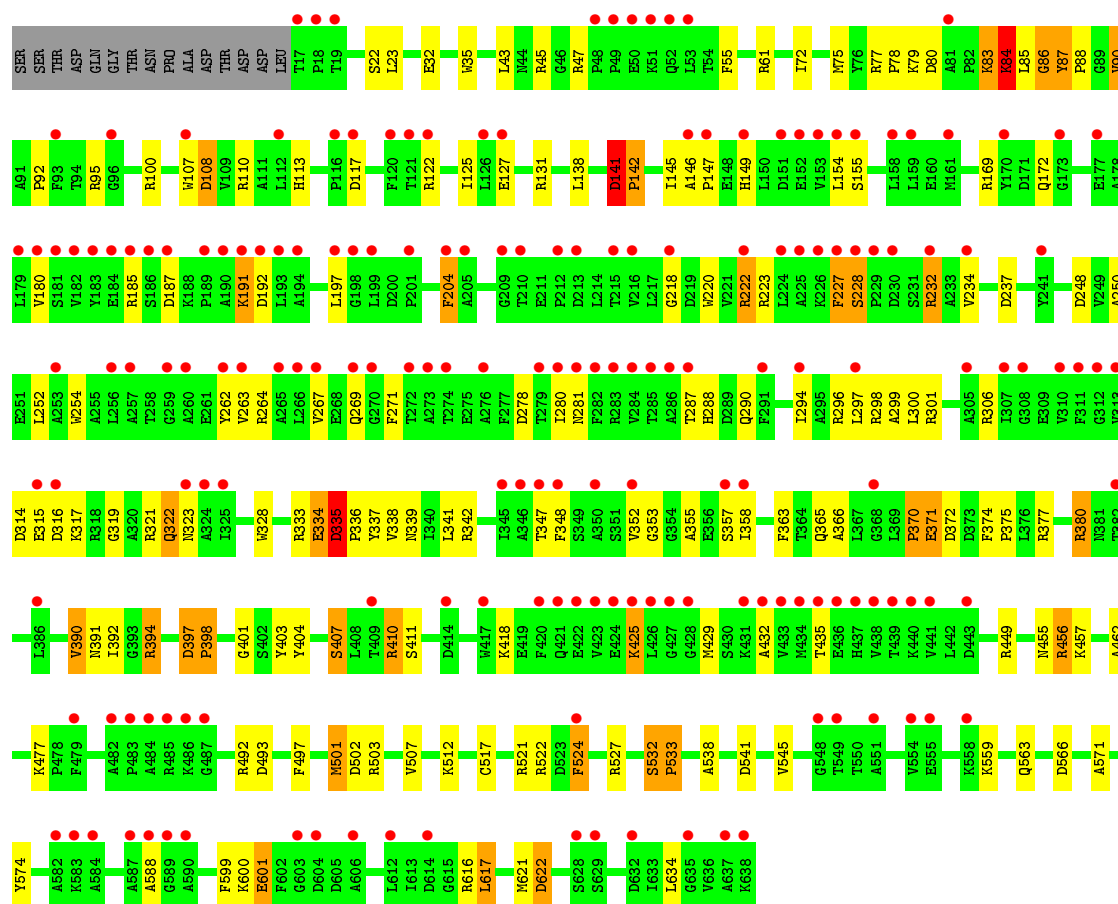


• Molecule 2: METHYLMALONYL-COA MUTASE



• Molecule 2: METHYLMALONYL-COA MUTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.80 Å 161.30 Å 88.40 Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 39.62 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 96.0 (39.62-1.97)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.87 (at 1.97 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.275 0.252 , 0.271	Depositor DCC
R_{free} test set	10913 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 74.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	0 of 217311 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22372	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, B12, DCA

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	0.91	0/5679	2.03	166/7718 (2.2%)
1	C	0.95	1/5676 (0.0%)	2.14	199/7711 (2.6%)
2	B	0.82	0/4785	2.04	136/6499 (2.1%)
2	D	0.76	0/4783	2.06	143/6503 (2.2%)
All	All	0.87	1/20923 (0.0%)	2.07	644/28431 (2.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25
1	C	0	37
2	B	0	21
2	D	0	17
All	All	0	100

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	558	ARG	NE-CZ	5.04	1.39	1.33

The worst 5 of 644 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	264	ARG	CD-NE-CZ	38.96	178.14	123.60
2	D	169	ARG	CD-NE-CZ	30.40	166.16	123.60
1	C	384	ARG	CD-NE-CZ	25.54	159.35	123.60
1	A	384	ARG	CD-NE-CZ	24.99	158.59	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	723	ARG	NE-CZ-NH1	21.19	130.90	120.30

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	THR	Mainchain
1	A	41	ALA	Mainchain
1	A	61	LEU	Mainchain
1	A	70	PHE	Mainchain
1	A	87	ARG	Mainchain

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	5563	0	5443	41	0
1	C	5560	0	5456	49	0
2	B	4695	0	4610	40	0
2	D	4692	0	4580	48	0
3	A	91	0	88	11	0
3	C	91	0	88	10	0
4	A	47	0	32	0	0
4	C	47	0	32	0	0
5	A	12	0	16	3	0
5	B	18	0	24	2	0
5	C	12	0	16	3	0
5	D	12	0	15	1	0
6	A	457	0	0	0	0
6	B	318	0	0	1	0
6	C	493	0	0	2	0
6	D	264	0	0	1	0
All	All	22372	0	20400	178	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 4.

The worst 5 of 178 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)
3:A:800:B12:H363	3:A:800:B12:C42	1.54	1.29
3:A:800:B12:C36	3:A:800:B12:H421	1.67	1.23
3:A:800:B12:H531	3:A:800:B12:H552	1.24	1.10
3:A:800:B12:H372	3:A:800:B12:H351	1.51	0.90
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.20	0.89

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	725/727 (100%)	698 (96%)	26 (4%)	1 (0%)	56	53
1	C	725/727 (100%)	685 (94%)	37 (5%)	3 (0%)	39	33
2	B	617/637 (97%)	595 (96%)	21 (3%)	1 (0%)	52	48
2	D	620/637 (97%)	580 (94%)	38 (6%)	2 (0%)	46	41
All	All	2687/2728 (98%)	2558 (95%)	122 (4%)	7 (0%)	46	41

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	ALA
1	C	16	PRO
2	D	228	SER
1	A	486	SER
1	C	486	SER

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	571/590 (97%)	550 (96%)	21 (4%)	41	38
1	C	571/590 (97%)	551 (96%)	20 (4%)	43	40
2	B	474/509 (93%)	455 (96%)	19 (4%)	38	33
2	D	472/509 (93%)	448 (95%)	24 (5%)	29	23
All	All	2088/2198 (95%)	2004 (96%)	84 (4%)	38	33

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	586	LYS
1	C	287	PHE
2	D	411	SER
2	B	629	SER
1	C	52	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	322	GLN
1	C	191	GLN
2	D	322	GLN
2	B	323	ASN
2	B	391	ASN

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 [i](#)

13 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	B12	A	800	1	74,101,101	1.44	12 (16%)	111,166,166	2.03	29 (26%)
4	DCA	A	801	-	39,49,49	1.12	2 (5%)	50,74,74	1.45	7 (14%)
5	GOL	A	802	-	5,5,5	0.82	0	5,5,5	1.68	1 (20%)
5	GOL	A	803	-	5,5,5	0.80	0	5,5,5	0.63	0
5	GOL	B	1	-	5,5,5	0.64	0	5,5,5	0.27	0
5	GOL	B	639	-	5,5,5	0.37	0	5,5,5	0.56	0
5	GOL	B	640	-	5,5,5	0.42	0	5,5,5	0.36	0
3	B12	C	800	1,6	74,101,101	1.41	6 (8%)	111,166,166	2.29	43 (38%)
4	DCA	C	801	-	39,49,49	1.31	5 (12%)	50,74,74	1.72	11 (22%)
5	GOL	C	802	-	5,5,5	1.10	0	5,5,5	2.75	1 (20%)
5	GOL	C	803	-	5,5,5	0.50	0	5,5,5	0.59	0
5	GOL	D	1	-	5,5,5	0.69	0	5,5,5	2.09	1 (20%)
5	GOL	D	639	-	5,5,5	0.24	0	5,5,5	0.86	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	B12	A	800	1	-	0/51/223/223	0/3/11/11
4	DCA	A	801	-	-	0/43/63/63	0/3/3/3
5	GOL	A	802	-	-	0/4/4/4	0/0/0/0
5	GOL	A	803	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	639	-	-	0/4/4/4	0/0/0/0
5	GOL	B	640	-	-	0/4/4/4	0/0/0/0
3	B12	C	800	1,6	-	0/51/223/223	0/3/11/11
4	DCA	C	801	-	-	0/43/63/63	0/3/3/3
5	GOL	C	802	-	-	0/4/4/4	0/0/0/0
5	GOL	C	803	-	-	0/4/4/4	0/0/0/0
5	GOL	D	1	-	-	0/4/4/4	0/0/0/0
5	GOL	D	639	-	-	0/4/4/4	0/0/0/0

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	C17-C18	-3.00	1.50	1.54
4	C	801	DCA	P1A-O1A	-2.45	1.42	1.51
4	C	801	DCA	CDP-CBP	-2.33	1.48	1.53
4	A	801	DCA	P2A-O5A	-2.32	1.45	1.54
3	A	800	B12	O2-C3R	-2.32	1.37	1.44

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C13-C14-C15	-5.36	113.80	131.88
3	A	800	B12	C55-C56-C57	-5.35	100.25	111.06
3	C	800	B12	C2P-C1P-N59	-5.25	105.15	112.92
3	A	800	B12	C13-C14-C15	-4.84	115.54	131.88
3	A	800	B12	C2P-C1P-N59	-4.80	105.81	112.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	B12	11	0
5	A	802	GOL	3	0
5	B	639	GOL	1	0
5	B	640	GOL	1	0
3	C	800	B12	10	0
5	C	802	GOL	3	0
5	D	1	GOL	1	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	727/727 (100%)	0.88	41 (5%) 28 29	19, 35, 61, 89	0
1	C	727/727 (100%)	0.99	63 (8%) 13 13	18, 34, 60, 105	0
2	B	619/637 (97%)	1.00	69 (11%) 7 8	23, 41, 61, 82	0
2	D	622/637 (97%)	1.52	181 (29%) 1 1	23, 50, 75, 103	0
All	All	2695/2728 (98%)	1.08	354 (13%) 5 5	18, 39, 67, 105	0

The worst 5 of 354 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	THR	8.1
2	D	428	GLY	8.1
2	D	190	ALA	7.4
1	C	30	ALA	7.0
1	A	3	THR	6.6

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
5	GOL	B	1	6/6	0.52	0.38	8.25	54,59,61,61	0
5	GOL	D	639	6/6	0.74	0.29	7.60	53,61,64,70	0
5	GOL	B	640	6/6	0.70	0.29	7.41	50,60,62,68	0
5	GOL	D	1	6/6	0.61	0.28	1.93	61,62,64,68	0
5	GOL	A	802	6/6	0.88	0.21	0.98	29,41,45,48	0
5	GOL	B	639	6/6	0.81	0.20	0.88	44,48,53,53	0
3	B12	C	800	91/91	0.95	0.18	0.55	15,26,40,53	0
5	GOL	C	803	6/6	0.89	0.19	0.49	38,39,41,45	0
5	GOL	C	802	6/6	0.88	0.20	0.48	21,32,43,45	0
3	B12	A	800	91/91	0.95	0.17	0.32	17,29,48,68	0
5	GOL	A	803	6/6	0.91	0.17	0.19	34,38,42,46	0
4	DCA	C	801	47/47	0.93	0.16	-0.40	14,23,30,32	0
4	DCA	A	801	47/47	0.94	0.16	-0.60	20,25,28,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.