



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

PDB ID : 1DIO  
Title : DIOL DEHYDRATASE-CYANOCOBALAMIN COMPLEX FROM KLEBSIELLA OXYTOCA  
Authors : Shibata, N.; Masuda, J.; Tobimatsu, T.; Toraya, T.; Suto, K.; Morimoto, Y.; Yasuoka, N.  
Deposited on : 1999-01-27  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

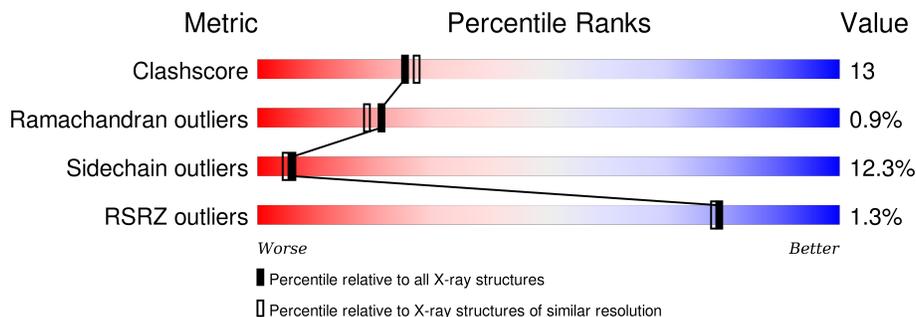
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	554	 66% 27% 6% ..
1	L	554	 66% 27% 6% ..
2	B	224	 52% 21% 7% 20%
2	E	224	 6% 43% 28% 6% • 20%
3	G	173	 45% 28% 6% • 21%
3	M	173	 2% 51% 21% 6% • 21%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	PGO	A	602	-	-	-	X
6	PGO	L	602	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13912 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 PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	551	4201	2620	727	825	29	0	0	0
1	L	551	4201	2620	727	825	29	0	0	0

- Molecule 2 is a protein called PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	179	1367	865	245	255	2	0	0	0
2	E	179	1367	865	245	255	2	0	0	0

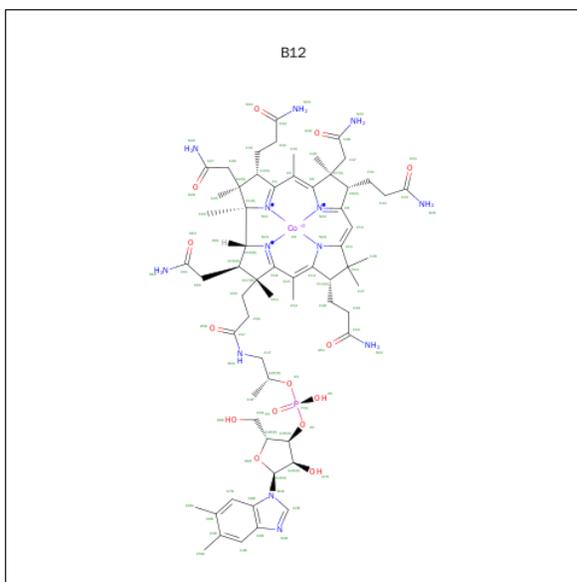
- Molecule 3 is a protein called PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	137	1093	681	195	214	3	0	0	0
3	M	137	1093	681	195	214	3	0	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

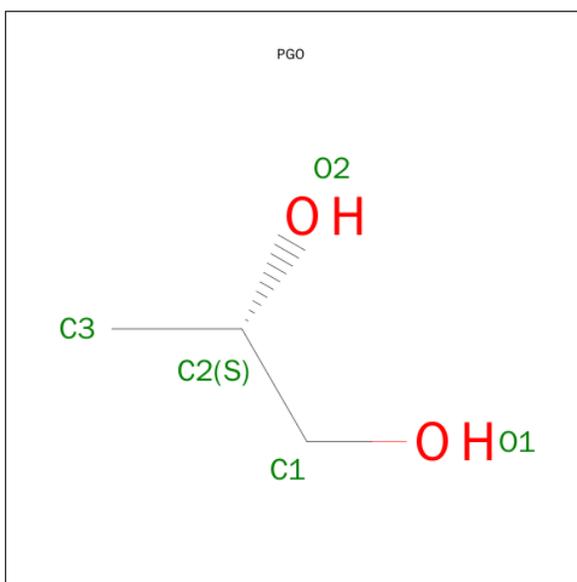
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total 1 K 1	0	0
4	L	1	Total 1 K 1	0	0

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
5	B	1	91	62	1	13	14	1	0	0
5	E	1	91	62	1	13	14	1	0	0

- Molecule 6 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula:  $C_3H_8O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
6	A	1	5	3 2	0	0
6	L	1	5	3 2	0	0

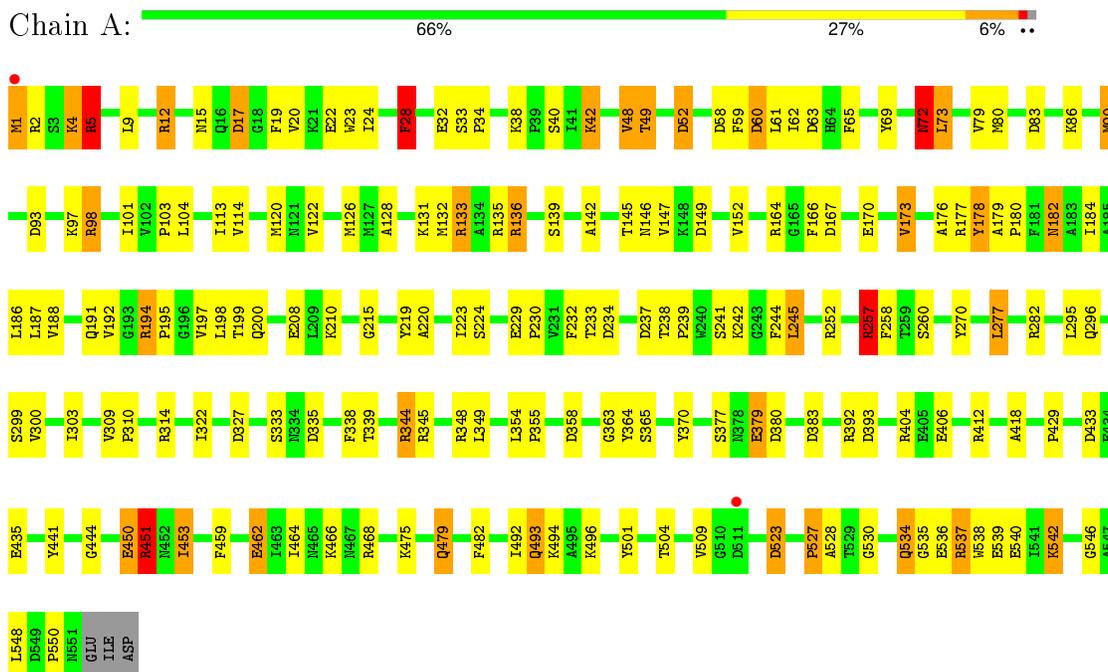
- Molecule 7 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	A	144	Total 144	O 144	0	0
7	B	41	Total 41	O 41	0	0
7	E	22	Total 22	O 22	0	0
7	G	24	Total 24	O 24	0	0
7	L	150	Total 150	O 150	0	0
7	M	15	Total 15	O 15	0	0

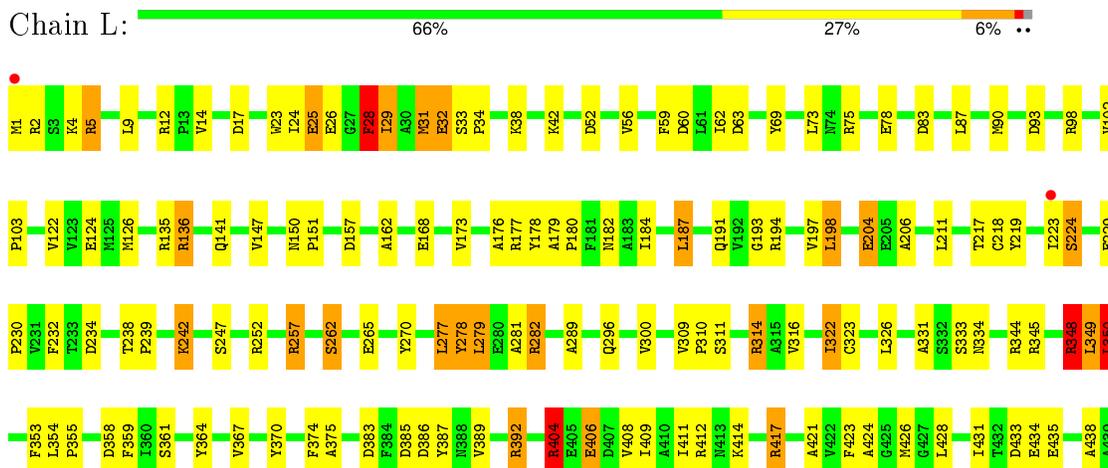
### 3 Residue-property plots

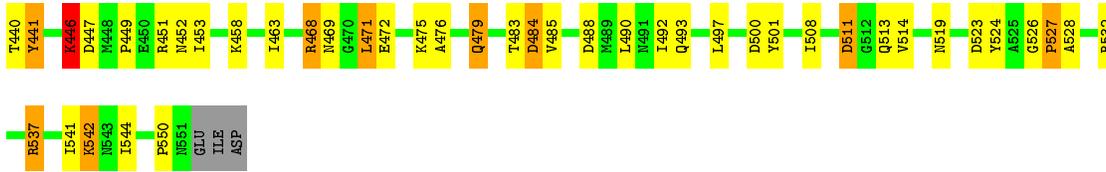
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PROTEIN (DIOL DEHYDRATASE)

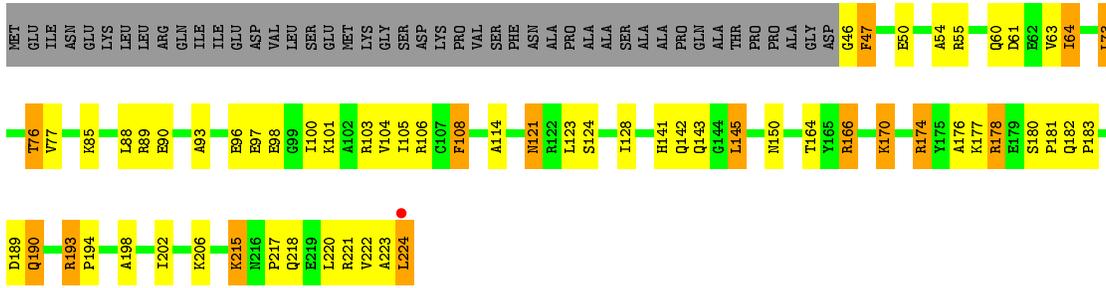


- Molecule 1: PROTEIN (DIOL DEHYDRATASE)

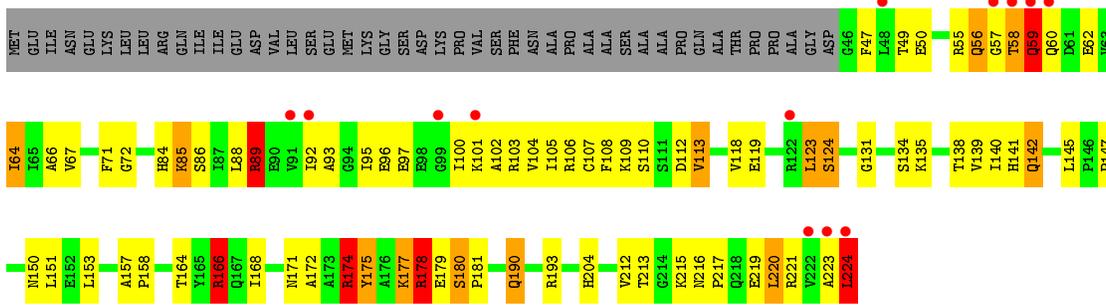




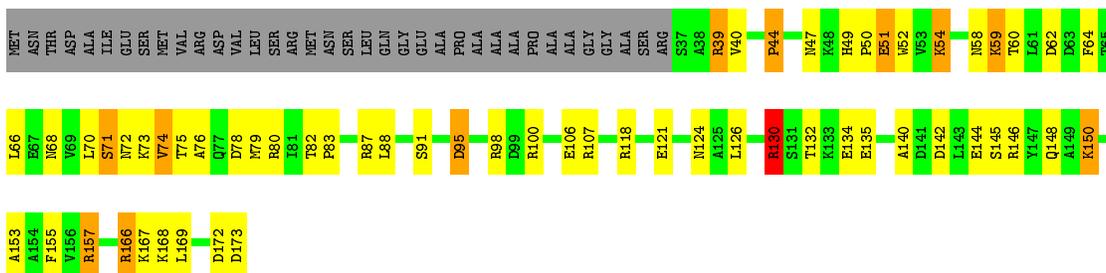
- Molecule 2: PROTEIN (DIOL DEHYDRATASE)



- Molecule 2: PROTEIN (DIOL DEHYDRATASE)



- Molecule 3: PROTEIN (DIOL DEHYDRATASE)



- Molecule 3: PROTEIN (DIOL DEHYDRATASE)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.20Å 122.30Å 209.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 47.46 – 2.17	Depositor EDS
% Data completeness (in resolution range)	83.5 (10.00-2.20) 83.5 (47.46-2.17)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.16Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.187 , 0.236 0.170 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.633	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Outliers	0 of 87366 reflections	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: PGO, K, B12

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	0.74	0/4273	1.82	87/5787 (1.5%)
1	L	0.69	0/4273	1.67	73/5787 (1.3%)
2	B	0.58	0/1389	1.51	15/1879 (0.8%)
2	E	0.52	0/1389	1.48	13/1879 (0.7%)
3	G	0.62	0/1108	1.77	18/1497 (1.2%)
3	M	0.57	0/1108	1.71	19/1497 (1.3%)
All	All	0.67	0/13540	1.70	225/18326 (1.2%)

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	1	1
1	L	0	1
All	All	1	2

There are no bond length outliers.

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ARG	NE-CZ-NH1	28.38	134.49	120.30
1	A	12	ARG	NE-CZ-NH2	-19.58	110.51	120.30
1	A	537	ARG	NE-CZ-NH2	-18.16	111.22	120.30
3	M	130	ARG	NE-CZ-NH2	-17.85	111.38	120.30
1	A	83	ASP	CB-CG-OD1	16.12	132.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ALA	Mainchain
1	L	322	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	4201	0	4140	92	0
1	L	4201	0	4140	83	0
2	B	1367	0	1419	43	0
2	E	1367	0	1419	51	0
3	G	1093	0	1101	38	0
3	M	1093	0	1101	33	0
4	A	1	0	0	0	0
4	L	1	0	0	0	0
5	B	91	0	88	6	0
5	E	91	0	88	9	0
6	A	5	0	6	1	0
6	L	5	0	5	1	0
7	A	144	0	0	2	0
7	B	41	0	0	1	0
7	E	22	0	0	3	0
7	G	24	0	0	1	0
7	L	150	0	0	2	0
7	M	15	0	0	0	0
All	All	13912	0	13507	340	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 13.

The worst 5 of 340 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:M:59:LYS:HE3	3:M:60:THR:H	1.20	1.01
2:B:76:THR:HG22	2:B:77:VAL:HG13	1.39	1.00
2:E:64:ILE:HG13	2:E:124:SER:HB2	1.41	1.00
3:M:59:LYS:HE2	3:M:63:ASP:HB2	1.46	0.93
2:E:179:GLU:O	2:E:180:SER:HB2	1.67	0.91

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	549/554 (99%)	512 (93%)	33 (6%)	4 (1%)	26	25
1	L	549/554 (99%)	508 (92%)	37 (7%)	4 (1%)	26	25
2	B	177/224 (79%)	171 (97%)	6 (3%)	0	100	100
2	E	177/224 (79%)	155 (88%)	16 (9%)	6 (3%)	5	2
3	G	135/173 (78%)	130 (96%)	5 (4%)	0	100	100
3	M	135/173 (78%)	128 (95%)	6 (4%)	1 (1%)	26	25
All	All	1722/1902 (90%)	1604 (93%)	103 (6%)	15 (1%)	21	19

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	180	SER
1	L	2	ARG
1	L	446	LYS
2	E	59	GLN
2	E	178	ARG

### 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	450/453 (99%)	405 (90%)	45 (10%)	9	8
1	L	450/453 (99%)	400 (89%)	50 (11%)	8	6
2	B	147/183 (80%)	127 (86%)	20 (14%)	5	3
2	E	147/183 (80%)	118 (80%)	29 (20%)	1	1
3	G	116/141 (82%)	101 (87%)	15 (13%)	5	4
3	M	116/141 (82%)	100 (86%)	16 (14%)	4	3
All	All	1426/1554 (92%)	1251 (88%)	175 (12%)	6	5

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	167	LYS
1	L	218	CYS
3	M	54	LYS
1	L	9	LEU
1	L	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	68	ASN
1	L	72	ASN
2	E	216	ASN
1	L	15	ASN
1	L	74	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
6	PGO	A	602	4	4,4,4	0.48	0	2,4,4	0.97	0
5	B12	B	601	-	74,101,101	1.23	6 (8%)	111,166,166	2.01	30 (27%)
5	B12	E	601	-	74,101,101	1.07	7 (9%)	111,166,166	1.85	27 (24%)
6	PGO	L	602	4	4,4,4	0.54	0	2,4,4	1.70	1 (50%)

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
6	PGO	A	602	4	-	0/2/2/2	0/0/0/0
5	B12	B	601	-	-	0/51/223/223	0/3/11/11
5	B12	E	601	-	-	0/51/223/223	0/3/11/11
6	PGO	L	602	4	-	0/2/2/2	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	601	B12	P-O5	-2.64	1.42	1.48
5	B	601	B12	C60-C18	-2.10	1.49	1.54

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	B12	C20-C1	-2.10	1.49	1.53
5	B	601	B12	C8B-N1B	-2.05	1.36	1.38
5	E	601	B12	P-O4	2.12	1.54	1.48

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	B12	O2-P-O3	-6.89	93.51	100.07
5	E	601	B12	O2-P-O3	-6.83	93.57	100.07
5	B	601	B12	O58-C57-C56	-6.80	110.25	121.98
5	E	601	B12	O58-C57-C56	-5.30	112.84	121.98
5	B	601	B12	C7B-C8B-C9B	-4.61	115.98	120.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	PGO	1	0
5	B	601	B12	6	0
5	E	601	B12	9	0
6	L	602	PGO	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, 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	551/554 (99%)	-0.59	2 (0%) 93 93	13, 24, 52, 90	0
1	L	551/554 (99%)	-0.50	2 (0%) 93 93	11, 27, 54, 76	0
2	B	179/224 (79%)	-0.67	1 (0%) 90 90	18, 37, 64, 99	0
2	E	179/224 (79%)	0.29	13 (7%) 18 17	21, 45, 82, 117	0
3	G	137/173 (79%)	-0.56	0 100 100	24, 35, 65, 78	0
3	M	137/173 (79%)	-0.39	4 (2%) 55 54	25, 37, 73, 86	0
All	All	1734/1902 (91%)	-0.46	22 (1%) 79 78	11, 31, 62, 117	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	58	ASN	4.4
2	E	224	LEU	3.9
2	E	58	THR	3.8
2	E	222	VAL	3.7
1	L	1	MET	3.6

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	PGO	A	602	5/5	0.95	0.26	3.29	23,23,24,25	0
6	PGO	L	602	5/5	0.97	0.27	3.12	21,23,25,25	0
5	B12	B	601	91/91	0.97	0.14	0.65	17,23,27,40	0
5	B12	E	601	91/91	0.97	0.13	0.36	22,28,31,38	0
4	K	A	603	1/1	0.98	0.10	-2.04	18,18,18,18	0
4	K	L	603	1/1	0.98	0.10	-2.93	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.