



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:39 PM GMT

PDB ID : 1UJW  
Title : Structure of the complex between BtuB and Colicin E3 Receptor binding domain  
Authors : Kurisu, G.; Zakharov, S.D.; Zhalnina, M.V.; Bano, S.; Eroukova, V.Y.; Rokitskaya, T.I.; Antonenko, Y.N.; Wiener, M.C.; Cramer, W.A.  
Deposited on : 2003-08-12  
Resolution : 2.75 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

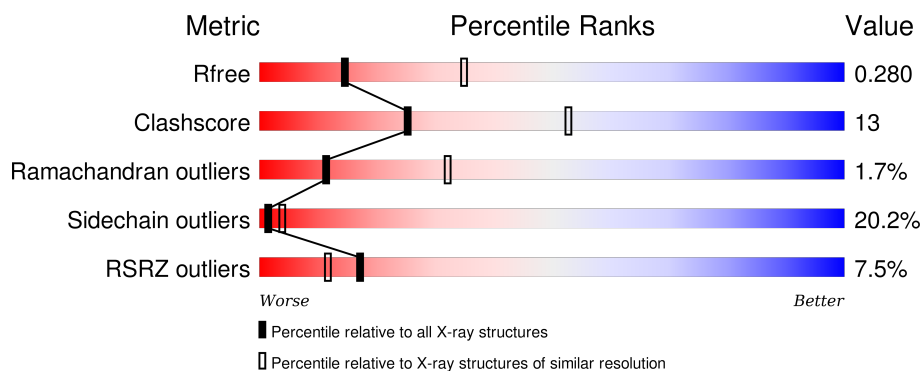
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	594	<div> <div>5%</div> <div>61%</div> <div>26%</div> <div>9%</div> <div>• •</div> </div>
2	B	135	<div> <div>18%</div> <div>59%</div> <div>21%</div> <div>5%</div> <div>•</div> <div>14%</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
3	GP1	A	801	-	-	-	X
4	LIM	A	812	-	-	-	X
5	LDA	A	601	-	-	-	X
5	LDA	A	603	-	-	-	X
5	LDA	A	604	-	-	-	X
5	LDA	A	605	-	-	-	X
5	LDA	A	606	-	-	-	X
5	LDA	A	607	-	-	-	X
7	LIM	A	803	-	-	-	X
8	GOL	A	701	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5714 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.

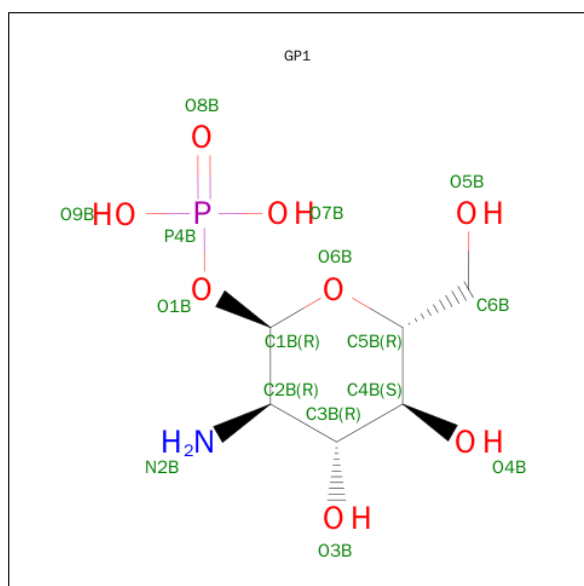
- Molecule 1 is a protein called Vitamin B12 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4567	2877	781	907	2			

- Molecule 2 is a protein called Colicin E3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			905	546	177	178	4			

- Molecule 3 is SUGAR (GLUCOSAMINE 1-PHOSPHATE) (three-letter code: GP1) (formula:  $C_6H_{14}NO_8P$ ).

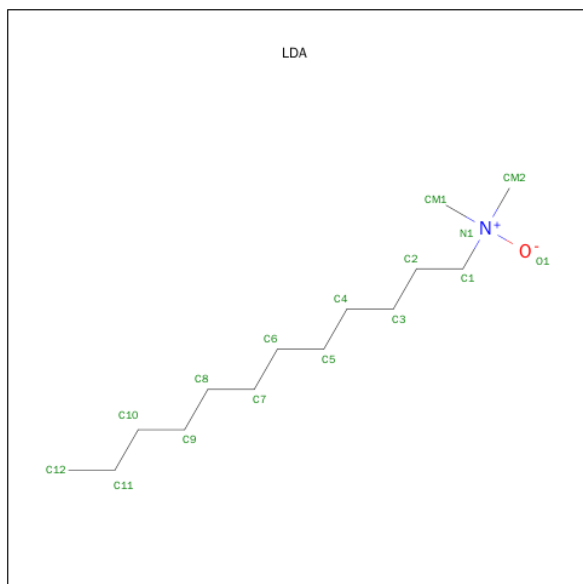


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

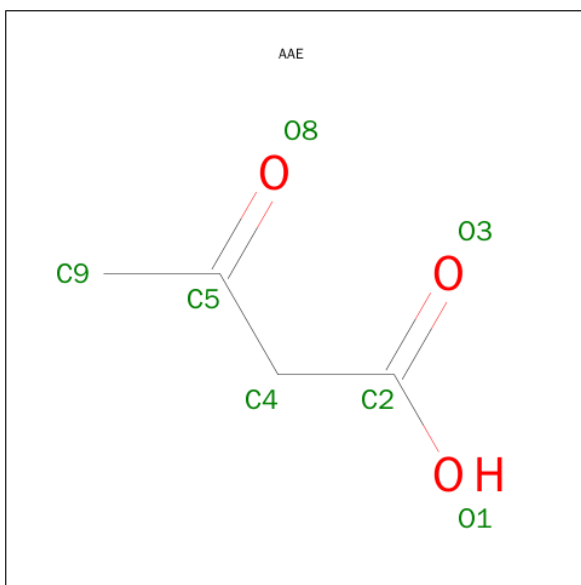
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	2	Total	C	N	O	P	0	0
			33	21	1	10	1		

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



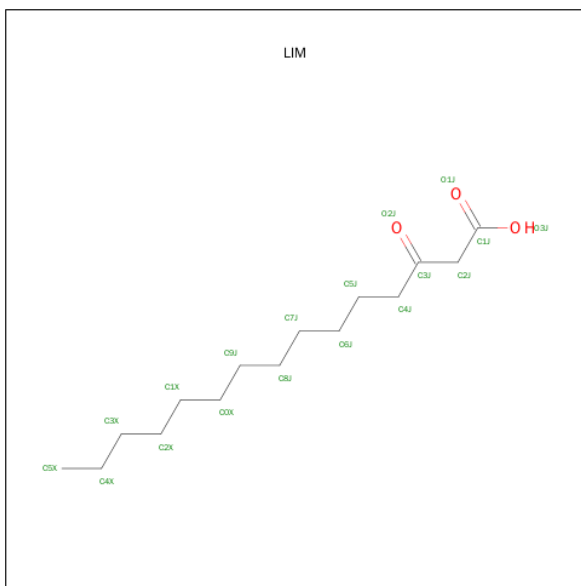
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O		0	0
			16	14	1	1			
5	A	1	Total	C	N	O		0	0
			16	14	1	1			
5	A	1	Total	C	N	O		0	0
			16	14	1	1			
5	A	1	Total	C	N	O		0	0
			16	14	1	1			
5	A	1	Total	C	N	O		0	0
			16	14	1	1			
5	A	1	Total	C	N	O		0	0
			16	14	1	1			

- Molecule 6 is ACETOACETIC ACID (three-letter code: AAE) (formula:  $C_4H_6O_3$ ).



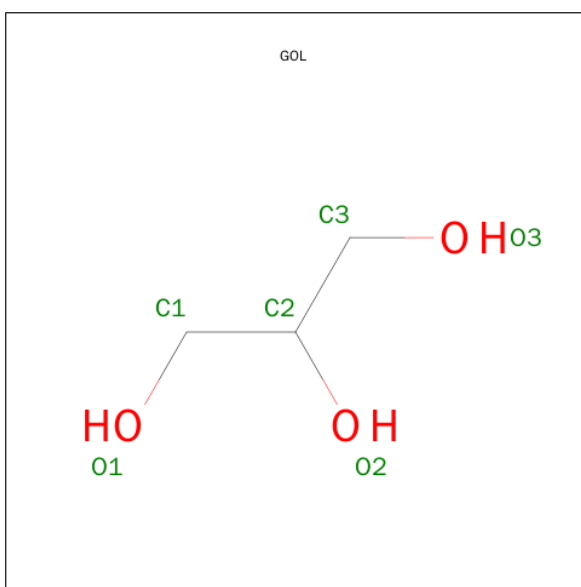
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is 3-OXO-PENTADECANOIC ACID (three-letter code: LIM) (formula:  $C_{15}H_{28}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	9	Total O 9 9	0	0
9	B	1	Total O 1 1	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.93Å 80.10Å 233.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.88 – 2.75 37.88 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.7 (37.88-2.75) 96.8 (37.88-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.244 , 0.293 0.233 , 0.280	Depositor DCC
$R_{free}$ test set	1864 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.9	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.4	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 37144 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5714	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AAE, GOL, LDA, GP1, LIM

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	0.81	1/4684 (0.0%)	1.03	27/6377 (0.4%)
2	B	0.61	0/914	0.86	4/1220 (0.3%)
All	All	0.78	1/5598 (0.0%)	1.01	31/7597 (0.4%)

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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	GLU	CG-CD	6.04	1.61	1.51

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASP	CB-CG-OD2	8.96	126.36	118.30
1	A	492	ASP	CB-CG-OD2	8.19	125.67	118.30
1	A	33	ASP	CB-CG-OD2	8.13	125.62	118.30
2	B	336	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	230	ASP	CB-CG-OD2	7.00	124.60	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	LEU	Peptide
1	A	229	TYR	Peptide
1	A	474	PRO	Peptide

## 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	4567	0	4287	133	0
2	B	905	0	885	9	0
3	A	16	0	10	1	0
4	A	33	0	37	1	0
5	A	112	0	217	6	0
6	A	6	0	5	1	0
7	A	17	0	27	1	0
8	A	48	0	63	5	0
9	A	9	0	0	2	0
9	B	1	0	0	0	0
All	All	5714	0	5531	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 13.

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)
1:A:13:ASN:H	1:A:13:ASN:HD22	1.10	1.00
1:A:506:GLN:HA	1:A:506:GLN:HE21	1.41	0.86
1:A:506:GLN:HE22	1:A:519:THR:HB	1.40	0.85
1:A:506:GLN:NE2	1:A:519:THR:HB	1.92	0.84
1:A:556:THR:HG21	8:A:708:GOL:O2	1.76	0.83

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	572/594 (96%)	525 (92%)	36 (6%)	11 (2%)	10	28
2	B	114/135 (84%)	111 (97%)	2 (2%)	1 (1%)	21	52
All	All	686/729 (94%)	636 (93%)	38 (6%)	12 (2%)	11	32

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	539	VAL
1	A	197	PHE
1	A	283	ARG
1	A	363	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	481/495 (97%)	391 (81%)	90 (19%)	2	5
2	B	88/104 (85%)	63 (72%)	25 (28%)	0	1
All	All	569/599 (95%)	454 (80%)	115 (20%)	1	4

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	THR

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Mol	Chain	Res	Type
1	A	451	LEU
2	B	388	ARG
1	A	384	ARG
1	A	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	372	GLN
2	B	401	GLN
1	A	362	ASN
1	A	400	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 ⓘ

2 carbohydrates 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$
4	GP1	A	811	4	15,16,16	1.14	1 (6%)	20,24,24	2.94	8 (40%)
4	LIM	A	812	4	16,16,17	3.14	3 (18%)	13,16,18	2.25	3 (23%)

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
4	GP1	A	811	4	-	0/6/27/27	0/1/1/1
4	LIM	A	812	4	-	0/14/15/16	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	811	GP1	C4B-C3B	2.04	1.57	1.52
4	A	812	LIM	C2J-C3J	3.55	1.56	1.52
4	A	812	LIM	O1J-C1J	3.86	1.44	1.19
4	A	812	LIM	O2J-C3J	11.18	1.42	1.21

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	812	LIM	O2J-C3J-C2J	-6.06	110.48	120.82
4	A	811	GP1	O6B-C1B-O1B	-5.30	104.38	111.36
4	A	812	LIM	O2J-C3J-C4J	-4.46	107.07	121.16
4	A	811	GP1	O1B-P4B-O8B	-3.70	97.87	107.11
4	A	812	LIM	C5J-C4J-C3J	-2.23	109.69	115.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	812	LIM	1	0

## 5.6 Ligand geometry ⓘ

18 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
5	LDA	A	601	-	15,15,15	3.64	1 (6%)	16,17,17	1.37	3 (18%)
5	LDA	A	602	-	15,15,15	3.75	2 (13%)	16,17,17	1.39	1 (6%)
5	LDA	A	603	-	15,15,15	3.24	1 (6%)	16,17,17	0.68	0
5	LDA	A	604	-	15,15,15	3.15	1 (6%)	16,17,17	1.26	3 (18%)
5	LDA	A	605	-	15,15,15	3.36	1 (6%)	16,17,17	1.02	2 (12%)
5	LDA	A	606	-	15,15,15	3.06	1 (6%)	16,17,17	1.27	1 (6%)
5	LDA	A	607	-	15,15,15	2.79	2 (13%)	16,17,17	1.06	1 (6%)
8	GOL	A	701	-	5,5,5	0.57	0	5,5,5	0.52	0
8	GOL	A	702	-	5,5,5	0.74	0	5,5,5	0.87	0
8	GOL	A	703	-	5,5,5	0.48	0	5,5,5	0.52	0
8	GOL	A	704	-	5,5,5	0.76	0	5,5,5	0.92	0
8	GOL	A	705	-	5,5,5	0.47	0	5,5,5	0.45	0
8	GOL	A	706	-	5,5,5	0.56	0	5,5,5	0.73	0
8	GOL	A	707	-	5,5,5	0.49	0	5,5,5	0.81	0
8	GOL	A	708	-	5,5,5	0.40	0	5,5,5	0.29	0
3	GP1	A	801	7,6	15,16,16	1.00	1 (6%)	20,24,24	3.56	9 (45%)
6	AAE	A	802	3	5,5,6	3.48	3 (60%)	3,5,7	2.99	2 (66%)
7	LIM	A	803	3	16,16,17	3.18	2 (12%)	13,16,18	1.83	2 (15%)

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
5	LDA	A	601	-	-	0/13/13/13	0/0/0/0
5	LDA	A	602	-	-	0/13/13/13	0/0/0/0
5	LDA	A	603	-	-	0/13/13/13	0/0/0/0
5	LDA	A	604	-	-	0/13/13/13	0/0/0/0
5	LDA	A	605	-	-	0/13/13/13	0/0/0/0
5	LDA	A	606	-	-	0/13/13/13	0/0/0/0
5	LDA	A	607	-	-	0/13/13/13	0/0/0/0
8	GOL	A	701	-	-	0/4/4/4	0/0/0/0
8	GOL	A	702	-	-	0/4/4/4	0/0/0/0
8	GOL	A	703	-	-	0/4/4/4	0/0/0/0
8	GOL	A	704	-	-	0/4/4/4	0/0/0/0
8	GOL	A	705	-	-	0/4/4/4	0/0/0/0
8	GOL	A	706	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	707	-	-	0/4/4/4	0/0/0/0
8	GOL	A	708	-	-	0/4/4/4	0/0/0/0
3	GP1	A	801	7,6	-	0/6/27/27	0/1/1/1
6	AAE	A	802	3	-	0/2/3/4	0/0/0/0
7	LIM	A	803	3	-	0/14/15/16	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	LDA	O1-N1	-14.30	1.26	1.39
5	A	601	LDA	O1-N1	-13.94	1.26	1.39
5	A	605	LDA	O1-N1	-12.79	1.27	1.39
5	A	603	LDA	O1-N1	-12.36	1.27	1.39
5	A	604	LDA	O1-N1	-12.04	1.28	1.39

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	GP1	O6B-C1B-O1B	-9.29	99.11	111.36
7	A	803	LIM	O2J-C3J-C2J	-4.71	112.79	120.82
5	A	602	LDA	O1-N1-C1	-4.21	105.54	110.27
6	A	802	AAE	O8-C5-C9	-4.16	111.05	121.31
7	A	803	LIM	O2J-C3J-C4J	-3.97	108.60	121.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	LDA	1	0
5	A	604	LDA	4	0
5	A	606	LDA	1	0
8	A	704	GOL	2	0
8	A	706	GOL	1	0
8	A	708	GOL	2	0
3	A	801	GP1	1	0
6	A	802	AAE	1	0
7	A	803	LIM	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	576/594 (96%)	0.33	28 (4%) 33 26	22, 32, 40, 51	0
2	B	116/135 (85%)	0.99	24 (20%) 1 1	30, 35, 39, 41	0
All	All	692/729 (94%)	0.44	52 (7%) 17 12	22, 32, 40, 51	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	325	ARG	6.3
1	A	573	TYR	5.1
2	B	326	ALA	4.9
2	B	323	TYR	4.6
1	A	194	ASN	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](#)

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
4	LIM	A	812	17/18	0.74	0.59	7.62	66,71,84,86	0
4	GP1	A	811	16/16	0.81	0.53	-	84,87,95,95	0

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GP1	A	801	16/16	0.72	0.38	7.38	77,83,91,91	0
5	LDA	A	607	16/16	0.81	0.39	7.16	53,65,75,75	0
7	LIM	A	803	17/18	0.84	0.28	4.33	63,69,76,77	0
5	LDA	A	605	16/16	0.78	0.36	4.20	67,70,76,78	0
8	GOL	A	701	6/6	0.93	0.42	3.29	62,64,64,65	0
5	LDA	A	601	16/16	0.85	0.32	2.92	59,65,68,69	0
5	LDA	A	606	16/16	0.86	0.30	2.60	53,56,62,63	0
5	LDA	A	603	16/16	0.95	0.27	2.57	53,55,65,65	0
5	LDA	A	604	16/16	0.92	0.31	2.05	60,64,69,70	0
5	LDA	A	602	16/16	0.91	0.28	1.25	52,57,64,66	0
8	GOL	A	706	6/6	0.72	0.19	0.40	61,65,68,69	0
8	GOL	A	702	6/6	0.90	0.24	0.27	56,58,59,60	0
8	GOL	A	704	6/6	0.95	0.16	-0.94	51,55,59,62	0
8	GOL	A	703	6/6	0.88	0.25	-	64,67,69,72	0
8	GOL	A	705	6/6	0.77	0.29	-	73,75,75,76	0
8	GOL	A	708	6/6	0.90	0.26	-	69,72,72,75	0
6	AAE	A	802	6/7	0.76	0.45	-	80,81,84,86	0
8	GOL	A	707	6/6	0.70	0.24	-	76,77,78,78	0

## 6.5 Other polymers

There are no such residues in this entry.