



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:14 PM GMT

PDB ID : 4R9U  
Title : Structure of vitamin B12 transporter BtuCD in a nucleotide-bound outward facing state  
Authors : Korkhov, V.M.; Mireku, S.A.; Veprintsev, D.B.; Locher, K.P.  
Deposited on : 2014-09-08  
Resolution : 2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

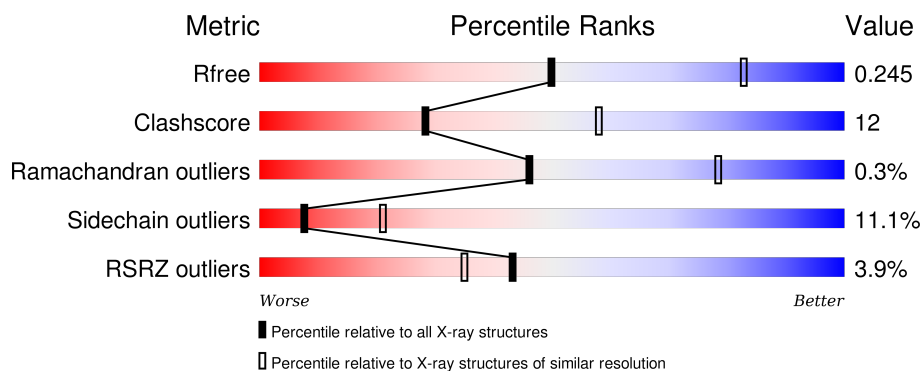
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	333	<div> <div>6%</div> <div>70% 24% . .</div> </div>
1	B	333	<div> <div>4%</div> <div>67% 26% 5% .</div> </div>
2	C	249	<div> <div>4%</div> <div>66% 30% .</div> </div>
2	D	249	<div> <div>%</div> <div>67% 29% .</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
3	LDA	A	502	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8792 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 import system permease protein BtuC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2441	1611	418	400	12			
1	B	324	Total	C	N	O	S	0	0	0
			2441	1611	418	400	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P06609
A	-5	PRO	-	EXPRESSION TAG	UNP P06609
A	-4	SER	-	EXPRESSION TAG	UNP P06609
A	-3	GLY	-	EXPRESSION TAG	UNP P06609
A	-2	THR	-	EXPRESSION TAG	UNP P06609
A	-1	SER	-	EXPRESSION TAG	UNP P06609
A	0	HIS	-	EXPRESSION TAG	UNP P06609
A	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	267	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	-6	GLY	-	EXPRESSION TAG	UNP P06609
B	-5	PRO	-	EXPRESSION TAG	UNP P06609
B	-4	SER	-	EXPRESSION TAG	UNP P06609
B	-3	GLY	-	EXPRESSION TAG	UNP P06609
B	-2	THR	-	EXPRESSION TAG	UNP P06609
B	-1	SER	-	EXPRESSION TAG	UNP P06609
B	0	HIS	-	EXPRESSION TAG	UNP P06609
B	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	156	SER	CYS	ENGINEERED MUTATION	UNP P06609

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Chain	Residue	Modelled	Actual	Comment	Reference
B	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	267	SER	CYS	ENGINEERED MUTATION	UNP P06609

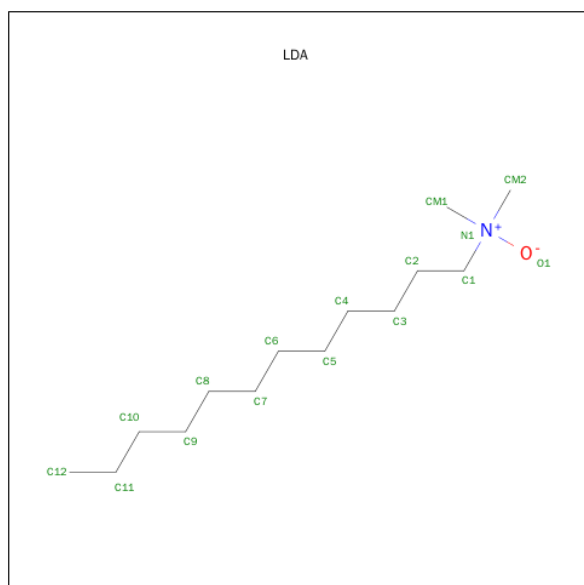
- Molecule 2 is a protein called Vitamin B12 import ATP-binding protein BtuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	248	Total	C	N	O	S	0	0	0
			1891	1183	351	348	9			
2	D	248	Total	C	N	O	S	0	0	0
			1891	1183	351	348	9			

There are 6 discrepancies between the modelled and reference sequences:

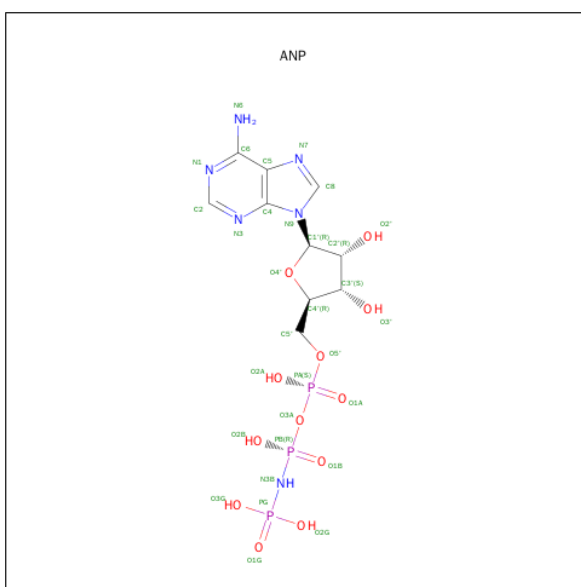
Chain	Residue	Modelled	Actual	Comment	Reference
C	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
C	162	CYS	ASN	ENGINEERED MUTATION	UNP P06611
C	180	SER	CYS	ENGINEERED MUTATION	UNP P06611
D	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
D	162	CYS	ASN	ENGINEERED MUTATION	UNP P06611
D	180	SER	CYS	ENGINEERED MUTATION	UNP P06611

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	D	1	Total 31	C 10	N 6	O 12	P 3	0	0

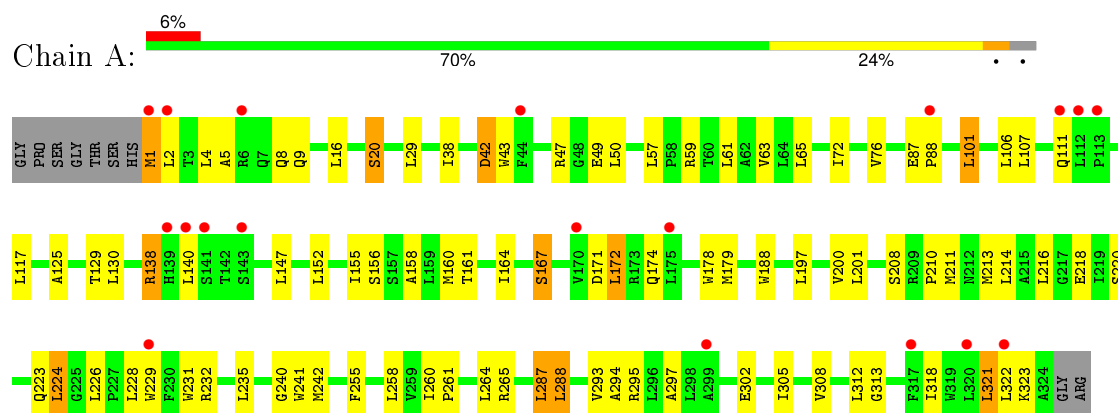
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

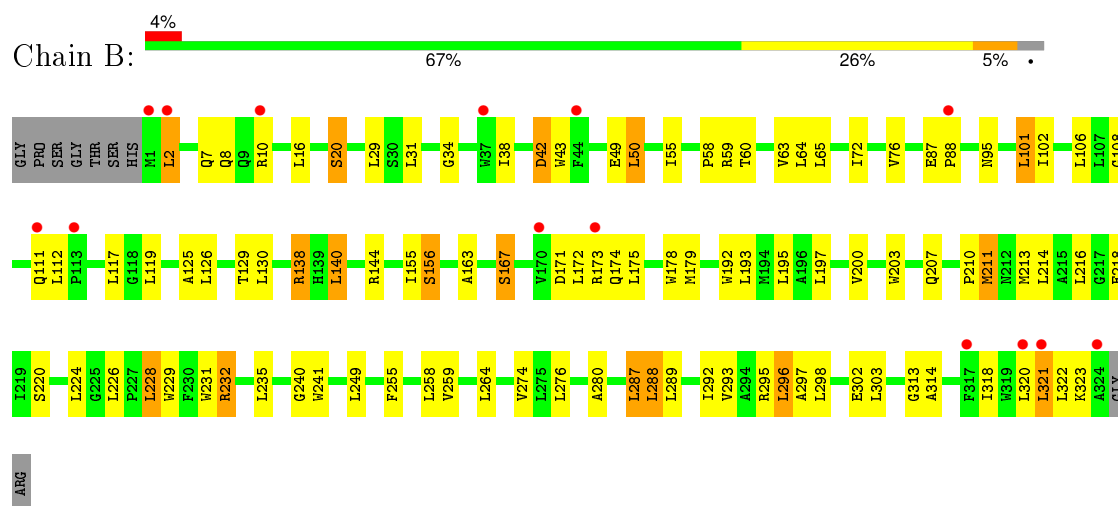
### 3 Residue-property plots

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.

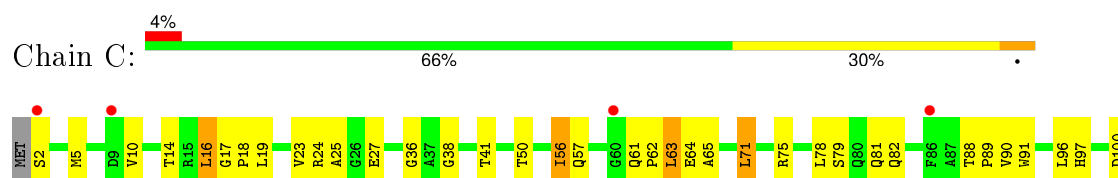
- Molecule 1: Vitamin B12 import system permease protein BtuC

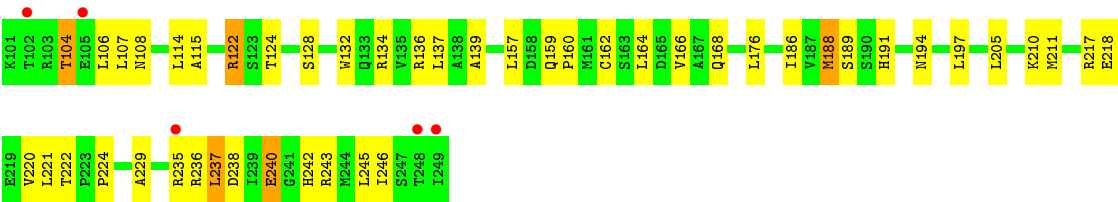


- Molecule 1: Vitamin B12 import system permease protein BtuC

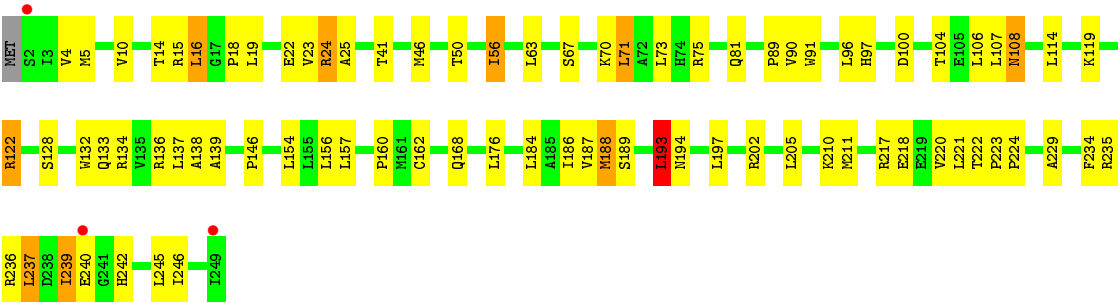


- Molecule 2: Vitamin B12 import ATP-binding protein BtuD





● Molecule 2: Vitamin B12 import ATP-binding protein BtuD





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	372.85Å 113.21Å 69.43Å 90.00° 94.92° 90.00°	Depositor
Resolution (Å)	29.51 – 2.79 29.51 – 2.79	Depositor EDS
% Data completeness (in resolution range)	69.2 (29.51-2.79) 69.2 (29.51-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.217 , 0.246 0.212 , 0.245	Depositor DCC
$R_{free}$ test set	1972 reflections (3.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 40.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 49831 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: MG, ANP, LDA

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	0.52	0/2495	0.75	2/3408 (0.1%)
1	B	0.53	0/2495	0.75	1/3408 (0.0%)
2	C	0.47	0/1925	0.67	0/2608
2	D	0.49	0/1925	0.74	2/2608 (0.1%)
All	All	0.51	0/8840	0.73	5/12032 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	193	LEU	CB-CG-CD2	-7.34	98.52	111.00
2	D	237	LEU	CB-CG-CD1	-6.88	99.30	111.00
1	A	50	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	B	228	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	A	260	ILE	C-N-CD	5.04	138.97	128.40

There are no chirality outliers.

There are no planarity outliers.

### 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	2441	0	2606	55	0
1	B	2441	0	2606	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1891	0	1924	49	0
2	D	1891	0	1924	47	0
3	A	32	0	62	1	0
3	B	32	0	62	1	0
4	C	31	0	13	3	0
4	D	31	0	13	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	8792	0	9210	209	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 12.

All (209) 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)
2:D:71:LEU:HD13	2:D:75:ARG:HH21	1.47	0.79
2:C:157:LEU:HB2	2:C:188:MET:HB3	1.65	0.78
1:B:34:GLY:HA2	1:B:296:LEU:HD22	1.65	0.78
1:A:224:LEU:HD21	2:C:97:HIS:HA	1.68	0.75
2:D:205:LEU:HD21	2:D:229:ALA:HB2	1.69	0.74
1:B:106:LEU:HD21	1:B:167:SER:HB3	1.69	0.74
1:B:129:THR:HG21	1:B:240:GLY:HA3	1.70	0.73
1:A:318:ILE:HG22	1:A:322:LEU:HG	1.69	0.72
2:C:205:LEU:HD21	2:C:229:ALA:HB2	1.70	0.72
1:A:322:LEU:O	1:B:138:ARG:NH1	2.22	0.71
2:D:5:MET:HB3	2:D:23:VAL:HB	1.72	0.71
1:B:200:VAL:HG21	1:B:241:TRP:CD1	2.27	0.70
2:C:71:LEU:HD13	2:C:75:ARG:HH21	1.56	0.69
1:A:106:LEU:HD21	1:A:167:SER:HB3	1.74	0.69
2:D:67:SER:OG	2:D:70:LYS:HG2	1.92	0.68
1:A:129:THR:HG21	1:A:240:GLY:HA3	1.74	0.68
1:A:318:ILE:HA	1:A:321:LEU:HD12	1.76	0.68
2:C:5:MET:HB3	2:C:23:VAL:HB	1.76	0.67
1:B:63:VAL:HG13	1:B:287:LEU:HD13	1.77	0.67
1:A:295:ARG:HA	1:A:302:GLU:HG3	1.76	0.66
1:B:214:LEU:HD21	1:B:228:LEU:HD21	1.78	0.66
2:D:222:THR:HG22	2:D:224:PRO:HD2	1.78	0.66
2:D:67:SER:H	2:D:70:LYS:HE2	1.59	0.65
2:C:17:GLY:HA3	2:C:210:LYS:HE3	1.76	0.65
1:B:60:THR:HG23	1:B:288:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:HA	1:B:302:GLU:HG3	1.78	0.64
1:A:57:LEU:HD23	1:A:188:TRP:HZ2	1.61	0.64
1:B:101:LEU:HD21	1:B:117:LEU:HB3	1.79	0.63
1:B:171:ASP:OD2	1:B:173:ARG:NH1	2.30	0.63
2:C:56:ILE:HD11	2:C:63:LEU:HD22	1.81	0.63
1:A:255:PHE:CZ	1:A:313:GLY:HA3	2.35	0.62
1:A:294:ALA:HB2	1:A:308:VAL:HG11	1.81	0.62
1:A:322:LEU:HB3	1:A:323:LYS:HE3	1.82	0.61
1:B:213:MET:HE2	1:B:226:LEU:HB2	1.82	0.61
1:A:101:LEU:HD21	1:A:117:LEU:HB3	1.82	0.61
1:B:318:ILE:HA	1:B:321:LEU:HD12	1.83	0.60
1:B:193:LEU:HD12	1:B:249:LEU:HD13	1.84	0.60
1:A:42:ASP:OD2	1:A:42:ASP:N	2.35	0.60
2:D:137:LEU:HD21	2:D:160:PRO:HB2	1.83	0.59
1:B:318:ILE:HG22	1:B:322:LEU:HG	1.85	0.59
1:A:63:VAL:HG11	1:A:288:LEU:HA	1.86	0.58
2:C:137:LEU:HD21	2:C:160:PRO:HB2	1.84	0.58
1:B:108:GLY:HA3	1:B:112:LEU:HD11	1.83	0.58
2:C:197:LEU:HD13	2:C:221:LEU:HD12	1.85	0.58
2:C:218:GLU:OE2	2:C:243:ARG:NH1	2.37	0.57
1:B:322:LEU:HB3	1:B:323:LYS:HE3	1.86	0.57
1:B:111:GLN:NE2	1:B:111:GLN:O	2.38	0.57
2:D:5:MET:HE3	2:D:46:MET:HB3	1.86	0.57
1:A:213:MET:HE2	1:A:226:LEU:HB2	1.86	0.57
2:C:19:LEU:HD22	2:C:211:MET:HB2	1.86	0.56
1:A:200:VAL:HG21	1:A:241:TRP:CD1	2.40	0.56
2:D:157:LEU:HB2	2:D:188:MET:HB3	1.88	0.55
2:C:222:THR:HG22	2:C:224:PRO:HD2	1.88	0.55
2:C:166:VAL:HG21	2:D:193:LEU:HD21	1.88	0.55
1:B:87:GLU:HG3	1:B:258:LEU:HB2	1.89	0.55
1:A:59:ARG:O	1:A:63:VAL:HG23	2.07	0.54
1:A:218:GLU:HG2	1:A:228:LEU:HD11	1.90	0.54
1:B:95:ASN:HB3	1:B:156:SER:HB2	1.89	0.54
1:B:102:ILE:HG21	1:B:163:ALA:HB1	1.90	0.54
2:D:114:LEU:HD12	2:D:138:ALA:HB2	1.90	0.53
2:D:119:LYS:HG2	2:D:122:ARG:HH21	1.73	0.53
2:C:97:HIS:CG	2:C:139:ALA:HB1	2.42	0.53
1:A:155:ILE:HD11	1:B:318:ILE:HG13	1.89	0.53
1:A:138:ARG:NH1	1:B:322:LEU:O	2.38	0.53
2:C:246:ILE:HD13	2:D:242:HIS:CG	2.44	0.53
1:B:288:LEU:O	1:B:292:ILE:HG13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:N	1:B:42:ASP:OD2	2.41	0.53
1:A:318:ILE:HG13	1:B:155:ILE:HD11	1.91	0.53
2:D:239:ILE:N	2:D:239:ILE:HD13	2.24	0.52
1:B:65:LEU:HB3	1:B:197:LEU:HD23	1.92	0.52
2:D:176:LEU:HD22	2:D:186:ILE:HD13	1.93	0.51
2:C:194:ASN:OD1	2:C:245:LEU:N	2.43	0.51
2:D:132:TRP:CE2	2:D:136:ARG:HD2	2.45	0.51
1:B:72:ILE:HD11	1:B:280:ALA:HB2	1.92	0.51
1:A:59:ARG:NH2	1:A:302:GLU:OE2	2.35	0.51
1:B:108:GLY:HA3	1:B:112:LEU:CD1	2.41	0.50
1:A:5:ALA:O	1:A:9:GLN:HB2	2.11	0.50
1:A:308:VAL:O	1:A:312:LEU:HG	2.12	0.50
2:D:22:GLU:OE1	2:D:24:ARG:NH2	2.45	0.50
1:A:16:LEU:O	1:A:20:SER:OG	2.30	0.49
1:B:255:PHE:CZ	1:B:313:GLY:HA3	2.48	0.49
1:A:38:ILE:HG22	1:A:43:TRP:HD1	1.77	0.49
2:D:157:LEU:HB3	2:D:160:PRO:HG3	1.93	0.49
1:A:201:LEU:HG	1:A:242:MET:HE3	1.95	0.49
1:A:87:GLU:HG3	1:A:258:LEU:HB2	1.95	0.49
2:D:133:GLN:OE1	2:D:136:ARG:NH1	2.43	0.49
1:A:125:ALA:O	1:A:129:THR:HG23	2.13	0.48
1:B:178:TRP:HE3	1:B:179:MET:HG2	1.78	0.48
2:D:4:VAL:HG23	2:D:25:ALA:HB2	1.94	0.48
2:C:36:GLY:HA2	4:C:301:ANP:H3'	1.94	0.48
1:B:7:GLN:O	1:B:10:ARG:HG2	2.13	0.48
2:C:16:LEU:HD12	2:C:41:THR:HG22	1.95	0.48
2:D:22:GLU:O	2:D:202:ARG:NH2	2.47	0.48
1:A:4:LEU:HD13	2:C:91:TRP:CD1	2.49	0.47
2:D:18:PRO:HD2	2:D:210:LYS:HZ2	1.78	0.47
1:B:87:GLU:CG	1:B:258:LEU:HB2	2.44	0.47
1:B:289:LEU:O	1:B:293:VAL:HG23	2.14	0.47
1:A:171:ASP:HB3	1:A:174:GLN:HB2	1.96	0.47
2:C:61:GLN:HG2	2:C:62:PRO:HD2	1.95	0.47
2:D:220:VAL:HG12	2:D:221:LEU:HD23	1.96	0.47
2:C:2:SER:O	2:C:25:ALA:HB2	2.15	0.47
1:A:38:ILE:HG22	1:A:43:TRP:CD1	2.50	0.47
2:C:197:LEU:HD22	2:C:245:LEU:HD12	1.97	0.47
2:D:134:ARG:HD3	2:D:168:GLN:HG3	1.97	0.47
1:A:261:PRO:HB2	1:A:265:ARG:HH21	1.80	0.47
1:A:214:LEU:HD21	1:A:228:LEU:HD21	1.97	0.46
1:A:210:PRO:HG3	1:A:231:TRP:CZ2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.66	0.46
2:C:240:GLU:CD	2:D:235:ARG:HH12	2.18	0.46
2:C:237:LEU:HD21	2:C:246:ILE:HD12	1.98	0.46
1:A:76:VAL:HG13	1:A:235:LEU:HD13	1.98	0.46
1:A:287:LEU:HA	1:A:287:LEU:HD23	1.71	0.46
2:C:24:ARG:HB2	2:C:27:GLU:HG2	1.98	0.46
1:B:210:PRO:HG3	1:B:231:TRP:CZ2	2.51	0.46
2:D:205:LEU:HD21	2:D:229:ALA:CB	2.44	0.46
2:D:70:LYS:O	2:D:73:LEU:HB2	2.15	0.46
2:C:38:GLY:HA2	4:C:301:ANP:H5'1	1.98	0.46
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.71	0.45
1:B:218:GLU:HG2	1:B:228:LEU:HD11	1.99	0.45
2:D:19:LEU:HD22	2:D:211:MET:HB2	1.96	0.45
1:B:314:ALA:O	1:B:318:ILE:HG12	2.16	0.45
2:D:10:VAL:O	2:D:18:PRO:HA	2.17	0.45
1:B:264:LEU:HD23	1:B:264:LEU:HA	1.64	0.45
1:B:140:LEU:O	1:B:232:ARG:NH2	2.43	0.45
2:C:114:LEU:O	2:C:134:ARG:NH1	2.42	0.45
1:B:298:LEU:HB2	1:B:303:LEU:HD11	1.97	0.45
1:A:160:MET:O	1:A:164:ILE:HG13	2.16	0.45
1:B:59:ARG:NH2	1:B:302:GLU:OE2	2.36	0.45
3:A:501:LDA:HM12	3:A:501:LDA:H22	1.66	0.45
1:A:178:TRP:HE3	1:A:179:MET:HG2	1.81	0.45
1:A:147:LEU:HA	1:A:147:LEU:HD23	1.64	0.45
2:D:97:HIS:CG	2:D:139:ALA:HB1	2.52	0.45
1:B:125:ALA:O	1:B:129:THR:HG23	2.17	0.45
1:B:293:VAL:O	1:B:297:ALA:HB2	2.17	0.45
1:B:76:VAL:HG13	1:B:235:LEU:HD13	1.98	0.45
2:D:194:ASN:OD1	2:D:245:LEU:N	2.50	0.45
1:A:158:ALA:HA	1:A:161:THR:HG22	1.99	0.45
2:C:63:LEU:C	2:C:65:ALA:H	2.20	0.45
1:B:55:ILE:O	1:B:58:PRO:HD2	2.16	0.45
1:B:119:LEU:HA	1:B:119:LEU:HD12	1.76	0.45
2:C:134:ARG:HD3	2:C:168:GLN:HG3	1.98	0.44
1:B:224:LEU:HD23	1:B:224:LEU:HA	1.64	0.44
2:C:90:VAL:HG23	2:C:122:ARG:O	2.16	0.44
2:C:88:THR:O	2:C:124:THR:HG23	2.17	0.44
1:B:16:LEU:O	1:B:20:SER:OG	2.33	0.44
1:B:255:PHE:CE1	1:B:259:VAL:HG21	2.53	0.44
1:B:192:TRP:CE3	3:B:501:LDA:H52	2.53	0.44
1:A:213:MET:CE	1:A:226:LEU:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:HG2	1:A:228:LEU:CD1	2.47	0.44
1:B:2:LEU:HD23	2:D:108:ASN:HD21	1.83	0.44
2:C:132:TRP:CE2	2:C:136:ARG:HD2	2.53	0.44
2:D:16:LEU:HD12	2:D:41:THR:HG22	2.00	0.44
2:C:36:GLY:H	4:C:301:ANP:HNB1	1.66	0.44
1:A:152:LEU:HA	1:A:152:LEU:HD23	1.73	0.44
1:B:126:LEU:O	1:B:130:LEU:HB2	2.18	0.44
2:D:146:PRO:HG3	2:D:184:LEU:HD13	1.99	0.44
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.82	0.44
2:D:67:SER:N	2:D:70:LYS:HE2	2.31	0.43
2:D:156:LEU:HD23	2:D:187:VAL:HB	2.00	0.43
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.85	0.43
1:B:59:ARG:O	1:B:63:VAL:HG23	2.18	0.43
1:A:65:LEU:HB3	1:A:197:LEU:HD23	1.99	0.43
2:D:236:ARG:HB3	2:D:236:ARG:HE	1.63	0.43
1:B:140:LEU:HD23	1:B:144:ARG:HB3	2.00	0.43
1:B:38:ILE:HG22	1:B:43:TRP:HD1	1.83	0.43
1:A:172:LEU:H	1:A:172:LEU:HG	1.54	0.43
2:D:71:LEU:HD13	2:D:75:ARG:NH2	2.25	0.43
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.82	0.42
1:A:305:ILE:HG21	1:A:305:ILE:HD13	1.74	0.42
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.77	0.42
2:C:10:VAL:O	2:C:18:PRO:HA	2.19	0.42
2:D:89:PRO:HB2	2:D:91:TRP:CD1	2.54	0.42
2:C:63:LEU:O	2:C:65:ALA:N	2.46	0.42
1:B:102:ILE:HG21	1:B:163:ALA:CB	2.49	0.42
2:D:15:ARG:HB2	4:D:301:ANP:O4'	2.20	0.42
1:A:16:LEU:HD23	1:A:16:LEU:HA	1.94	0.42
1:B:64:LEU:HD21	1:B:288:LEU:HD12	2.01	0.41
2:D:154:LEU:HD21	2:D:156:LEU:HD21	2.02	0.41
1:B:38:ILE:HG22	1:B:43:TRP:CD1	2.55	0.41
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.84	0.41
2:D:56:ILE:HD11	2:D:63:LEU:HD22	2.02	0.41
2:D:223:PRO:HB3	2:D:234:PHE:O	2.19	0.41
2:D:70:LYS:HA	2:D:73:LEU:HD12	2.02	0.41
2:C:242:HIS:CG	2:D:246:ILE:HD13	2.55	0.41
1:B:211:MET:HE3	1:B:214:LEU:HD12	2.01	0.41
2:C:197:LEU:HD12	2:C:197:LEU:HA	1.84	0.41
2:C:82:GLN:HE21	2:C:136:ARG:HH21	1.67	0.41
2:C:164:LEU:HA	2:C:164:LEU:HD23	1.74	0.41
1:A:293:VAL:O	1:A:297:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:ALA:HB3	2:C:134:ARG:NH1	2.36	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.85	0.41
1:B:203:TRP:O	1:B:207:GLN:HG2	2.21	0.41
2:C:159:GLN:NE2	2:C:191:HIS:HD2	2.19	0.41
2:C:235:ARG:NH1	2:D:240:GLU:OE2	2.54	0.41
2:C:89:PRO:HB2	2:C:91:TRP:CD1	2.56	0.41
2:C:176:LEU:HD22	2:C:186:ILE:HD13	2.03	0.41
2:C:78:LEU:HD23	2:C:79:SER:O	2.21	0.41
2:C:71:LEU:HD23	2:C:71:LEU:HA	1.84	0.41
1:A:1:MET:H3	2:C:104:THR:HG22	1.85	0.41
1:B:50:LEU:O	1:B:50:LEU:HG	2.21	0.41
1:B:175:LEU:HA	1:B:175:LEU:HD23	1.82	0.40
2:C:220:VAL:HG12	2:C:221:LEU:HD23	2.03	0.40
2:D:90:VAL:HG23	2:D:122:ARG:O	2.21	0.40
1:B:293:VAL:HG12	1:B:293:VAL:O	2.21	0.40
1:B:197:LEU:HD12	1:B:197:LEU:HA	1.77	0.40
2:C:205:LEU:HD21	2:C:229:ALA:CB	2.45	0.40
1:A:72:ILE:HD12	1:A:201:LEU:HD23	2.04	0.40
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.88	0.40
1:B:173:ARG:HG3	1:B:174:GLN:N	2.36	0.40

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	322/333 (97%)	293 (91%)	28 (9%)	1 (0%)	46	78
1	B	322/333 (97%)	294 (91%)	27 (8%)	1 (0%)	46	78
2	C	246/249 (99%)	232 (94%)	13 (5%)	1 (0%)	39	73
2	D	246/249 (99%)	234 (95%)	12 (5%)	0	100	100
All	All	1136/1164 (98%)	1053 (93%)	80 (7%)	3 (0%)	46	78



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	GLU
1	A	88	PRO
1	B	88	PRO

### 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	249/255 (98%)	222 (89%)	27 (11%)	8	22
1	B	249/255 (98%)	224 (90%)	25 (10%)	9	25
2	C	200/201 (100%)	176 (88%)	24 (12%)	6	17
2	D	200/201 (100%)	176 (88%)	24 (12%)	6	17
All	All	898/912 (98%)	798 (89%)	100 (11%)	8	21

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LEU
1	A	8	GLN
1	A	20	SER
1	A	29	LEU
1	A	42	ASP
1	A	47	ARG
1	A	49	GLU
1	A	101	LEU
1	A	111	GLN
1	A	130	LEU
1	A	138	ARG
1	A	140	LEU
1	A	156	SER
1	A	167	SER
1	A	172	LEU
1	A	208	SER

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Mol	Chain	Res	Type
1	A	211	MET
1	A	216	LEU
1	A	220	SER
1	A	223	GLN
1	A	224	LEU
1	A	229	TRP
1	A	232	ARG
1	A	287	LEU
1	A	288	LEU
1	A	321	LEU
1	B	2	LEU
1	B	8	GLN
1	B	20	SER
1	B	29	LEU
1	B	42	ASP
1	B	49	GLU
1	B	50	LEU
1	B	101	LEU
1	B	138	ARG
1	B	140	LEU
1	B	156	SER
1	B	167	SER
1	B	172	LEU
1	B	195	LEU
1	B	211	MET
1	B	216	LEU
1	B	220	SER
1	B	229	TRP
1	B	232	ARG
1	B	274	VAL
1	B	287	LEU
1	B	288	LEU
1	B	296	LEU
1	B	320	LEU
1	B	321	LEU
2	C	14	THR
2	C	16	LEU
2	C	50	THR
2	C	56	ILE
2	C	57	GLN
2	C	63	LEU
2	C	71	LEU

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Mol	Chain	Res	Type
2	C	81	GLN
2	C	96	LEU
2	C	100	ASP
2	C	104	THR
2	C	106	LEU
2	C	107	LEU
2	C	108	ASN
2	C	122	ARG
2	C	128	SER
2	C	162	CYS
2	C	188	MET
2	C	189	SER
2	C	217	ARG
2	C	236	ARG
2	C	237	LEU
2	C	238	ASP
2	C	240	GLU
2	D	14	THR
2	D	16	LEU
2	D	24	ARG
2	D	50	THR
2	D	56	ILE
2	D	71	LEU
2	D	81	GLN
2	D	96	LEU
2	D	100	ASP
2	D	104	THR
2	D	106	LEU
2	D	107	LEU
2	D	108	ASN
2	D	122	ARG
2	D	128	SER
2	D	162	CYS
2	D	188	MET
2	D	189	SER
2	D	193	LEU
2	D	197	LEU
2	D	217	ARG
2	D	218	GLU
2	D	237	LEU
2	D	239	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	81	GLN
2	C	159	GLN
2	D	57	GLN
2	D	81	GLN
2	D	191	HIS

### 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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	LDA	A	501	-	15,15,15	3.76	2 (13%)	16,17,17	0.63	0
3	LDA	A	502	-	15,15,15	3.67	2 (13%)	16,17,17	0.53	0
3	LDA	B	501	-	15,15,15	3.77	2 (13%)	16,17,17	0.55	0
3	LDA	B	502	-	15,15,15	3.83	2 (13%)	16,17,17	0.85	0
4	ANP	C	301	5	27,33,33	1.22	3 (11%)	30,52,52	1.23	4 (13%)
4	ANP	D	301	5	27,33,33	1.20	4 (14%)	30,52,52	1.38	4 (13%)

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	LDA	A	501	-	-	0/13/13/13	0/0/0/0
3	LDA	A	502	-	-	0/13/13/13	0/0/0/0
3	LDA	B	501	-	-	0/13/13/13	0/0/0/0
3	LDA	B	502	-	-	0/13/13/13	0/0/0/0
4	ANP	C	301	5	-	1/12/38/38	0/3/3/3
4	ANP	D	301	5	-	1/12/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	LDA	O1-N1	-14.50	1.25	1.39
3	B	501	LDA	O1-N1	-14.25	1.26	1.39
3	A	501	LDA	O1-N1	-14.23	1.26	1.39
3	A	502	LDA	O1-N1	-13.85	1.26	1.39
3	A	501	LDA	C1-N1	-2.65	1.46	1.51
3	B	502	LDA	C1-N1	-2.53	1.46	1.51
3	A	502	LDA	C1-N1	-2.44	1.46	1.51
3	B	501	LDA	C1-N1	-2.42	1.47	1.51
4	D	301	ANP	PB-N3B	2.08	1.68	1.63
4	D	301	ANP	PG-O1G	2.16	1.48	1.46
4	C	301	ANP	PB-O1B	2.29	1.48	1.46
4	D	301	ANP	PG-N3B	2.40	1.69	1.63
4	C	301	ANP	PG-N3B	2.73	1.70	1.63
4	D	301	ANP	PB-O1B	3.79	1.50	1.46
4	C	301	ANP	PG-O1G	3.80	1.50	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	ANP	O1B-PB-N3B	-3.52	106.49	111.90
4	D	301	ANP	PA-O3A-PB	-3.06	122.39	132.67
4	D	301	ANP	O3G-PG-O1G	-3.02	105.47	113.49
4	D	301	ANP	O2G-PG-O1G	-2.72	106.25	113.49
4	C	301	ANP	O2G-PG-O1G	-2.36	107.22	113.49
4	C	301	ANP	O3G-PG-O1G	-2.25	107.50	113.49
4	C	301	ANP	O2B-PB-O3A	2.01	114.22	105.09
4	D	301	ANP	O3G-PG-O2G	2.43	114.79	107.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	ANP	O1B-PB-N3B-PG
4	D	301	ANP	O1B-PB-N3B-PG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	LDA	1	0
3	B	501	LDA	1	0
4	C	301	ANP	3	0
4	D	301	ANP	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	324/333 (97%)	0.05	19 (5%) 26 18	41, 74, 140, 187	0
1	B	324/333 (97%)	-0.02	14 (4%) 39 31	37, 70, 137, 178	0
2	C	248/249 (99%)	0.09	9 (3%) 46 39	45, 88, 131, 193	0
2	D	248/249 (99%)	-0.15	3 (1%) 81 75	47, 76, 119, 200	0
All	All	1144/1164 (98%)	-0.00	45 (3%) 43 35	37, 75, 134, 200	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.4
2	D	249	ILE	6.1
2	C	249	ILE	6.1
2	C	2	SER	4.8
1	A	113	PRO	4.7
1	A	6	ARG	4.2
1	A	2	LEU	3.7
1	A	111	GLN	3.4
1	B	113	PRO	3.4
1	A	1	MET	3.4
1	B	321	LEU	3.2
1	B	44	PHE	3.1
1	B	111	GLN	2.9
1	A	139	HIS	2.8
1	B	2	LEU	2.8
1	B	324	ALA	2.7
1	A	140	LEU	2.7
1	A	170	VAL	2.7
1	A	299	ALA	2.7
1	A	317	PHE	2.6
1	A	88	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	2.5
2	C	235	ARG	2.5
2	C	102	THR	2.5
1	A	141	SER	2.5
1	A	229	TRP	2.5
1	B	317	PHE	2.5
2	C	9	ASP	2.4
1	A	320	LEU	2.4
2	D	2	SER	2.3
2	C	60	GLY	2.3
1	B	37	TRP	2.3
1	B	170	VAL	2.3
2	C	248	THR	2.3
1	A	143	SER	2.3
2	C	105	GLU	2.3
1	B	10	ARG	2.3
1	B	88	PRO	2.2
1	A	112	LEU	2.1
1	B	173	ARG	2.1
2	C	86	PHE	2.1
1	A	44	PHE	2.0
2	D	240	GLU	2.0
1	A	175	LEU	2.0
1	B	320	LEU	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
3	LDA	A	502	16/16	0.84	0.59	18.93	83,113,130,132	0
4	ANP	D	301	31/31	0.96	0.16	0.29	20,69,100,111	0
4	ANP	C	301	31/31	0.94	0.16	-0.16	45,78,100,106	0
3	LDA	A	501	16/16	0.91	0.46	-	71,81,111,115	0
3	LDA	B	501	16/16	0.88	0.45	-	60,66,114,119	0
5	MG	C	302	1/1	0.91	0.21	-	44,44,44,44	0
5	MG	D	302	1/1	0.97	0.20	-	48,48,48,48	0
3	LDA	B	502	16/16	0.89	0.48	-	83,95,120,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.