



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 08:29 AM EST

PDB ID : 6C0Y  
Title : Lysinoalanine synthase, DurN, from duramycin biosynthesis bound to duramycin  
Authors : Cogan, D.P.; Nair, S.K.  
Deposited on : 2018-01-03  
Resolution : 1.66 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

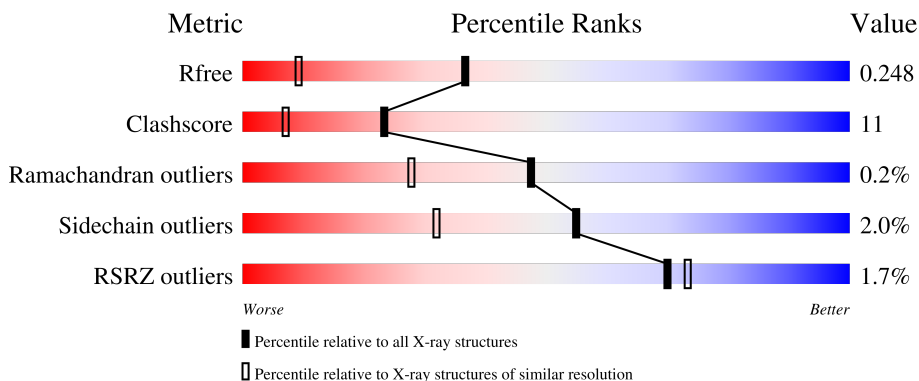
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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.



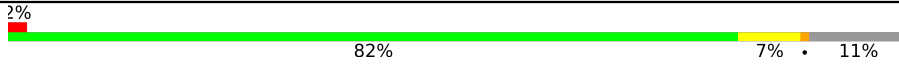

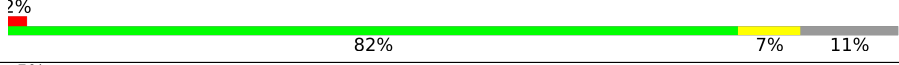
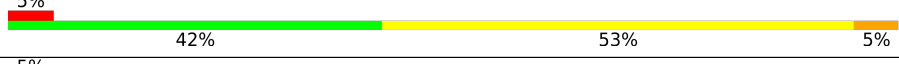
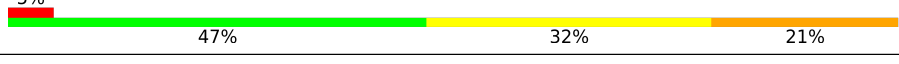
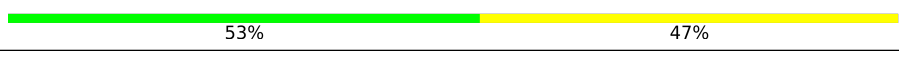
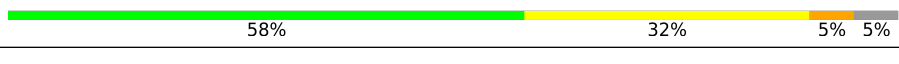
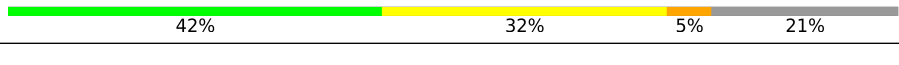
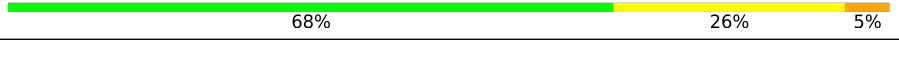

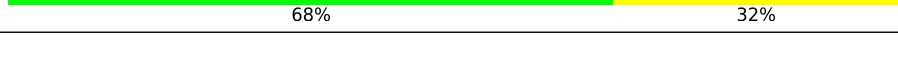
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	121	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">82%      6% • 12%</p>
1	B	121	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">73%      15% • 12%</p>
1	C	121	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">83%      6% • 11%</p>
1	D	121	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">75%      13% • 11%</p>
1	E	121	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81%      7% • 11%</p>

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Mol	Chain	Length	Quality of chain
1	F	121	
1	G	121	
1	H	121	
2	I	19	
2	J	19	
2	K	19	
2	L	19	
2	M	19	
2	N	19	
2	O	19	
2	P	19	

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
2	DBB	I	11	-	-	X	-
2	DAL	I	4	-	-	X	-
2	DBB	J	11	-	-	X	-
2	DAL	J	4	-	-	X	-
2	DBB	K	11	-	-	X	-
2	DBB	K	18	-	-	X	-
2	DAL	K	4	-	-	X	-
2	DBB	L	11	-	-	X	-
2	DBB	L	18	-	-	X	-
2	DAL	L	4	-	-	X	-
2	DBB	M	11	-	-	X	-
2	DAL	N	4	-	-	X	-
2	DBB	O	18	-	-	X	-
2	DAL	O	4	-	-	X	-
2	DBB	P	11	-	-	X	-
2	DAL	P	4	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9154 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 Lysinoalanine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	107	Total 841	C 534	N 146	O 158	S 3	0	1	0
1	B	107	Total 852	C 540	N 147	O 162	S 3	0	2	0
1	C	108	Total 880	C 555	N 156	O 166	S 3	0	4	0
1	D	108	Total 865	C 547	N 152	O 163	S 3	0	3	0
1	E	108	Total 855	C 540	N 151	O 161	S 3	0	2	0
1	F	108	Total 857	C 543	N 149	O 161	S 4	0	2	0
1	G	108	Total 851	C 539	N 147	O 162	S 3	0	1	0
1	H	108	Total 851	C 539	N 147	O 162	S 3	0	1	0

- Molecule 2 is a protein called CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	O	19	Total 140	C 89	N 23	O 25	S 3	0	0	0
2	I	19	Total 140	C 89	N 23	O 25	S 3	0	0	0
2	J	19	Total 136	C 86	N 22	O 25	S 3	0	0	0
2	K	19	Total 140	C 89	N 23	O 25	S 3	0	0	0
2	L	18	Total 130	C 83	N 21	O 23	S 3	0	0	0
2	M	15	Total 109	C 70	N 17	O 20	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	19	Total	C	N	O	S	0	0	0
			140	89	23	25	3			
2	P	19	Total	C	N	O	S	0	0	0
			136	86	22	25	3			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	B	2	Total	K	0	0
			2	2		
3	C	2	Total	K	0	0
			2	2		
3	D	2	Total	K	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	132	Total	O	0	0
			132	132		
4	C	166	Total	O	0	0
			166	166		
4	D	122	Total	O	0	0
			122	122		
4	E	119	Total	O	0	0
			119	119		
4	F	151	Total	O	0	0
			151	151		
4	G	148	Total	O	0	0
			148	148		
4	H	123	Total	O	0	0
			123	123		
4	O	16	Total	O	0	0
			16	16		
4	I	19	Total	O	0	0
			19	19		
4	J	16	Total	O	0	0
			16	16		

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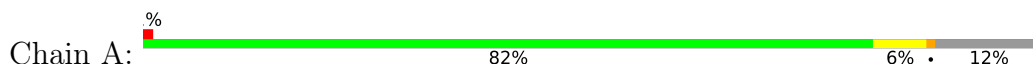
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	K	21	Total 21	O 21	0	0
4	L	17	Total 17	O 17	0	0
4	M	9	Total 9	O 9	0	0
4	N	20	Total 20	O 20	0	0
4	P	17	Total 17	O 17	0	0

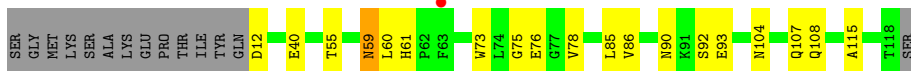
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

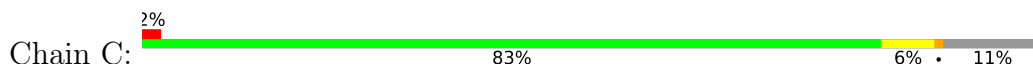
- Molecule 1: Lysinoalanine synthase



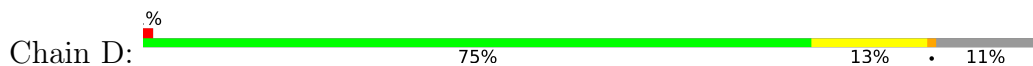
- Molecule 1: Lysinoalanine synthase



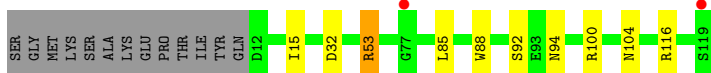
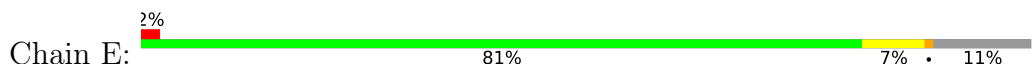
- Molecule 1: Lysinoalanine synthase



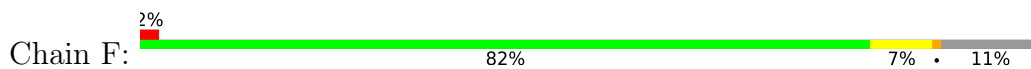
- Molecule 1: Lysinoalanine synthase



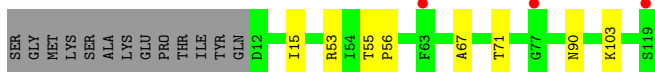
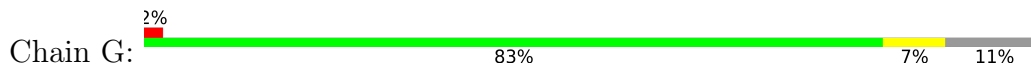
- Molecule 1: Lysinoalanine synthase



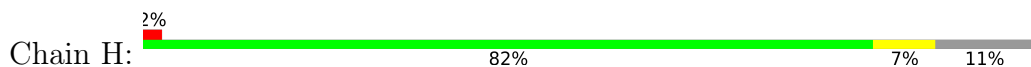
- Molecule 1: Lysinoalanine synthase



- Molecule 1: Lysinoalanine synthase



- Molecule 1: Lysinoalanine synthase



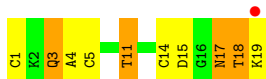
- Molecule 2: CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS



- Molecule 2: CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS



- Molecule 2: CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS



- Molecule 2: CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS







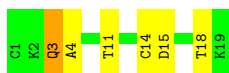
- Molecule 2: CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS



- Molecule 2: CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS



- Molecule 2: CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS



- Molecule 2: CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.88Å 67.42Å 69.12Å 71.51° 76.25° 72.92°	Depositor
Resolution (Å)	64.72 – 1.66 64.72 – 1.66	Depositor EDS
% Data completeness (in resolution range)	95.8 (64.72-1.66) 95.8 (64.72-1.66)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.66Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.184 , 0.242 0.198 , 0.248	Depositor DCC
$R_{free}$ test set	5255 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtrriage
Anisotropy	0.369	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9861e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: DBB, K, BH2, DAL

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	0.90	0/855	0.91	0/1162
1	B	1.04	0/866	1.00	0/1178
1	C	0.98	0/894	1.00	1/1214 (0.1%)
1	D	0.98	0/879	0.94	0/1194
1	E	0.97	0/869	1.05	2/1180 (0.2%)
1	F	1.01	0/871	0.99	0/1183
1	G	1.04	0/865	0.95	1/1175 (0.1%)
1	H	1.10	3/865 (0.3%)	1.05	5/1175 (0.4%)
2	I	1.29	1/113 (0.9%)	1.40	2/141 (1.4%)
2	J	1.12	0/109	1.14	0/137
2	K	1.05	0/113	1.17	0/141
2	L	1.32	0/104	1.03	0/133
2	M	1.27	0/89	1.12	0/114
2	N	1.15	0/113	1.28	0/141
2	O	1.24	0/113	1.20	0/141
2	P	1.16	0/109	1.11	0/137
All	All	1.03	4/7827 (0.1%)	1.01	11/10546 (0.1%)

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
2	I	0	1
2	J	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	75	GLY	N-CA	-8.24	1.33	1.46
1	H	75	GLY	CA-C	-7.66	1.39	1.51
1	H	84	GLU	CG-CD	6.04	1.61	1.51
2	I	19	LYS	N-CA	5.18	1.56	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	53	ARG	NE-CZ-NH1	-10.94	114.83	120.30
2	I	19	LYS	N-CA-C	7.41	131.01	111.00
1	G	53	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	H	53	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	H	53	ARG	NE-CZ-NH2	-6.62	116.99	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	17	ASN	Mainchain
2	J	17	ASN	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	841	0	863	9	0
1	B	852	0	874	16	0
1	C	880	0	903	6	0
1	D	865	0	886	15	0
1	E	855	0	871	8	0
1	F	857	0	877	6	0
1	G	851	0	872	6	0
1	H	851	0	872	7	0
2	I	140	0	128	21	0
2	J	136	0	117	15	0
2	K	140	0	131	26	0
2	L	130	0	118	16	0
2	M	109	0	91	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	140	0	124	8	0
2	O	140	0	129	21	0
2	P	136	0	117	9	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	127	0	0	4	0
4	B	132	0	0	2	0
4	C	166	0	0	3	0
4	D	122	0	0	7	0
4	E	119	0	0	2	0
4	F	151	0	0	0	0
4	G	148	0	0	1	0
4	H	123	0	0	1	0
4	I	19	0	0	0	0
4	J	16	0	0	0	0
4	K	21	0	0	0	0
4	L	17	0	0	0	0
4	M	9	0	0	1	0
4	N	20	0	0	0	0
4	O	16	0	0	0	0
4	P	17	0	0	0	0
All	All	9154	0	7973	180	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 11.

The worst 5 of 180 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:P:4:DAL:HB3	2:P:14:CYS:SG	1.19	1.75
2:K:5:CYS:SG	2:K:11:DBB:HB2	1.24	1.73
2:I:4:DAL:HB3	2:I:14:CYS:SG	1.17	1.71
2:L:5:CYS:SG	2:L:11:DBB:HB2	1.20	1.71
2:N:4:DAL:HB3	2:N:14:CYS:SG	1.18	1.69

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	106/121 (88%)	106 (100%)	0	0	100	100
1	B	107/121 (88%)	107 (100%)	0	0	100	100
1	C	110/121 (91%)	110 (100%)	0	0	100	100
1	D	109/121 (90%)	108 (99%)	0	1 (1%)	17	4
1	E	108/121 (89%)	108 (100%)	0	0	100	100
1	F	108/121 (89%)	107 (99%)	0	1 (1%)	17	4
1	G	107/121 (88%)	107 (100%)	0	0	100	100
1	H	107/121 (88%)	107 (100%)	0	0	100	100
2	I	13/19 (68%)	11 (85%)	2 (15%)	0	100	100
2	J	13/19 (68%)	13 (100%)	0	0	100	100
2	K	13/19 (68%)	13 (100%)	0	0	100	100
2	L	13/19 (68%)	13 (100%)	0	0	100	100
2	M	10/19 (53%)	9 (90%)	1 (10%)	0	100	100
2	N	13/19 (68%)	13 (100%)	0	0	100	100
2	O	13/19 (68%)	11 (85%)	2 (15%)	0	100	100
2	P	13/19 (68%)	12 (92%)	1 (8%)	0	100	100
All	All	963/1120 (86%)	955 (99%)	6 (1%)	2 (0%)	47	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	75	GLY
1	F	75	GLY

### 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	91/103 (88%)	89 (98%)	2 (2%)	52	27
1	B	93/103 (90%)	91 (98%)	2 (2%)	52	27
1	C	96/103 (93%)	95 (99%)	1 (1%)	76	62
1	D	94/103 (91%)	92 (98%)	2 (2%)	53	29
1	E	92/103 (89%)	89 (97%)	3 (3%)	38	12
1	F	93/103 (90%)	90 (97%)	3 (3%)	39	13
1	G	93/103 (90%)	93 (100%)	0	100	100
1	H	93/103 (90%)	93 (100%)	0	100	100
2	I	12/12 (100%)	12 (100%)	0	100	100
2	J	11/12 (92%)	10 (91%)	1 (9%)	9	1
2	K	12/12 (100%)	12 (100%)	0	100	100
2	L	11/12 (92%)	11 (100%)	0	100	100
2	M	9/12 (75%)	8 (89%)	1 (11%)	6	1
2	N	12/12 (100%)	11 (92%)	1 (8%)	11	2
2	O	12/12 (100%)	12 (100%)	0	100	100
2	P	11/12 (92%)	11 (100%)	0	100	100
All	All	835/920 (91%)	819 (98%)	16 (2%)	55	34

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	3	GLN
2	J	3	GLN
1	E	92	SER
1	F	108	GLN
1	E	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	108	GLN
1	G	90	ASN
2	M	17	ASN
2	J	3	GLN
1	D	108	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

31 non-standard protein/DNA/RNA residues 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
2	DBB	N	18	2	4,5,6	0.71	0	1,5,7	3.25	1 (100%)
2	DBB	N	11	2	4,5,6	1.13	1 (25%)	1,5,7	0.34	0
2	DBB	I	18	2	4,5,6	1.34	0	1,5,7	5.49	1 (100%)
2	DBB	K	11	2	4,5,6	0.83	0	1,5,7	1.78	0
2	BH2	P	15	2	6,8,9	1.61	2 (33%)	8,10,12	2.05	3 (37%)
2	DBB	P	18	2	4,5,6	1.09	0	1,5,7	4.00	1 (100%)
2	BH2	I	15	2	6,8,9	1.66	1 (16%)	8,10,12	1.82	3 (37%)
2	DBB	M	11	2	4,5,6	0.99	0	1,5,7	1.96	0
2	BH2	N	15	2	6,8,9	1.03	0	8,10,12	1.99	2 (25%)
2	BH2	K	15	2	6,8,9	0.97	0	8,10,12	2.17	3 (37%)
2	BH2	M	15	2	6,8,9	0.99	0	8,10,12	1.66	3 (37%)
2	BH2	L	15	2	6,8,9	1.54	1 (16%)	8,10,12	1.65	3 (37%)
2	DBB	O	11	2	4,5,6	0.06	0	1,5,7	0.51	0
2	BH2	O	15	2	6,8,9	1.20	0	8,10,12	1.65	2 (25%)
2	DBB	L	18	2	4,5,6	1.19	1 (25%)	1,5,7	0.50	0
2	DBB	J	18	2	4,5,6	1.56	1 (25%)	1,5,7	2.97	1 (100%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DBB	J	11	2	4,5,6	1.22	1 (25%)	1,5,7	0.31	0
2	DBB	I	11	2	4,5,6	0.82	0	1,5,7	1.48	0
2	DBB	O	18	2	4,5,6	0.52	0	1,5,7	1.94	0
2	DBB	L	11	2	4,5,6	0.14	0	1,5,7	0.45	0
2	DBB	P	11	2	4,5,6	0.24	0	1,5,7	0.15	0
2	BH2	J	15	2	6,8,9	1.53	1 (16%)	8,10,12	1.35	1 (12%)
2	DBB	K	18	2	4,5,6	1.03	0	1,5,7	0.56	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
2	DBB	N	18	2	-	0/3/4/6	-
2	DBB	N	11	2	-	1/3/4/6	-
2	DBB	I	18	2	-	0/3/4/6	-
2	DBB	K	11	2	-	1/3/4/6	-
2	BH2	P	15	2	-	1/9/10/12	-
2	DBB	P	18	2	-	1/3/4/6	-
2	BH2	I	15	2	-	3/9/10/12	-
2	DBB	M	11	2	-	2/3/4/6	-
2	BH2	N	15	2	-	2/9/10/12	-
2	BH2	K	15	2	-	2/9/10/12	-
2	BH2	M	15	2	-	3/9/10/12	-
2	BH2	L	15	2	-	1/9/10/12	-
2	DBB	O	11	2	-	0/3/4/6	-
2	BH2	O	15	2	-	3/9/10/12	-
2	DBB	L	18	2	-	1/3/4/6	-
2	DBB	J	18	2	-	2/3/4/6	-
2	DBB	J	11	2	-	1/3/4/6	-
2	DBB	I	11	2	-	1/3/4/6	-
2	DBB	O	18	2	-	2/3/4/6	-
2	DBB	L	11	2	-	1/3/4/6	-
2	DBB	P	11	2	-	1/3/4/6	-
2	BH2	J	15	2	-	3/9/10/12	-
2	DBB	K	18	2	-	0/3/4/6	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	15	BH2	OD1-CG	-3.33	1.19	1.30
2	L	15	BH2	OD1-CG	-2.65	1.21	1.30
2	J	15	BH2	CB-CG	-2.52	1.49	1.52
2	J	11	DBB	CA-N	-2.33	1.41	1.48
2	P	15	BH2	CA-N	-2.27	1.40	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	18	DBB	CG-CB-CA	-5.49	100.86	113.42
2	N	15	BH2	OD1-CG-OD2	-4.35	114.20	124.09
2	P	15	BH2	O-C-CA	-4.30	113.50	124.78
2	P	18	DBB	CG-CB-CA	-4.00	104.25	113.42
2	K	15	BH2	OD1-CG-OD2	-3.88	115.28	124.09

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	11	DBB	N-CA-CB-CG
2	J	11	DBB	N-CA-CB-CG
2	K	11	DBB	N-CA-CB-CG
2	L	11	DBB	N-CA-CB-CG
2	M	11	DBB	N-CA-CB-CG

There are no ring outliers.

10 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	11	DBB	5	0
2	M	11	DBB	8	0
2	L	18	DBB	6	0
2	J	18	DBB	1	0
2	J	11	DBB	7	0
2	I	11	DBB	5	0
2	O	18	DBB	5	0
2	L	11	DBB	5	0
2	P	11	DBB	5	0
2	K	18	DBB	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	107/121 (88%)	-0.25	1 (0%) 84 86	15, 23, 34, 39	0
1	B	107/121 (88%)	-0.34	1 (0%) 84 86	13, 19, 28, 40	0
1	C	108/121 (89%)	-0.29	2 (1%) 66 69	12, 17, 28, 46	0
1	D	108/121 (89%)	-0.15	1 (0%) 84 86	13, 19, 32, 50	0
1	E	108/121 (89%)	-0.14	2 (1%) 66 69	13, 22, 36, 53	0
1	F	108/121 (89%)	-0.25	3 (2%) 53 53	13, 18, 32, 48	0
1	G	108/121 (89%)	-0.32	3 (2%) 53 53	11, 17, 29, 42	0
1	H	108/121 (89%)	-0.23	2 (1%) 66 69	11, 19, 36, 55	0
2	I	15/19 (78%)	0.44	1 (6%) 17 16	17, 24, 34, 42	0
2	J	15/19 (78%)	0.50	1 (6%) 17 16	14, 22, 38, 48	0
2	K	15/19 (78%)	-0.15	0 100 100	14, 20, 26, 27	0
2	L	14/19 (73%)	-0.26	0 100 100	15, 18, 22, 26	0
2	M	12/19 (63%)	0.44	0 100 100	17, 23, 35, 37	0
2	N	15/19 (78%)	-0.03	0 100 100	15, 20, 31, 34	0
2	O	15/19 (78%)	-0.29	0 100 100	12, 18, 27, 27	0
2	P	15/19 (78%)	-0.26	0 100 100	13, 20, 29, 31	0
All	All	978/1120 (87%)	-0.21	17 (1%) 70 73	11, 20, 34, 55	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	16	GLY	4.8
1	D	119	SER	4.3
2	J	19	LYS	3.7
1	F	76	GLU	3.7
1	C	63	PHE	3.6

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	DBB	J	18	6/7	0.55	0.27	42,48,51,54	0
2	DBB	L	18	6/7	0.78	0.15	25,31,34,37	0
2	DBB	O	11	6/7	0.87	0.10	18,19,21,23	0
2	BH2	I	15	9/10	0.87	0.11	17,21,22,26	0
2	BH2	M	15	9/10	0.88	0.12	17,21,24,24	0
2	DBB	I	18	6/7	0.90	0.27	45,57,63,64	0
2	DBB	I	11	6/7	0.90	0.09	17,19,24,24	0
2	DBB	K	18	6/7	0.90	0.11	16,17,20,21	0
2	DBB	P	11	6/7	0.90	0.09	18,19,22,23	0
2	DBB	M	11	6/7	0.91	0.09	24,25,27,28	0
2	DBB	N	11	6/7	0.92	0.09	19,22,28,29	0
2	DAL	N	4	5/6	0.92	0.07	15,16,17,19	0
2	DBB	P	18	6/7	0.92	0.08	17,19,22,23	0
2	DBB	J	11	6/7	0.93	0.11	19,19,21,22	0
2	BH2	O	15	9/10	0.93	0.10	12,15,18,19	0
2	DAL	M	4	5/6	0.93	0.08	17,19,23,25	0
2	DAL	K	4	5/6	0.93	0.10	15,16,17,17	0
2	BH2	P	15	9/10	0.93	0.09	14,17,21,22	0
2	DBB	O	18	6/7	0.94	0.10	20,22,23,23	0
2	DBB	N	18	6/7	0.94	0.16	25,29,32,37	0
2	DAL	L	4	5/6	0.94	0.07	14,15,15,16	0
2	BH2	L	15	9/10	0.95	0.07	15,16,20,23	0
2	DBB	K	11	6/7	0.95	0.08	17,17,19,20	0
2	DAL	P	4	5/6	0.95	0.07	15,15,17,17	0
2	DAL	I	4	5/6	0.95	0.06	16,17,19,21	0
2	BH2	J	15	9/10	0.95	0.08	14,17,19,23	0
2	BH2	N	15	9/10	0.96	0.07	15,16,18,18	0
2	DBB	L	11	6/7	0.96	0.06	16,18,19,19	0
2	BH2	K	15	9/10	0.96	0.06	13,16,18,21	0
2	DAL	J	4	5/6	0.97	0.07	14,17,18,21	0
2	DAL	O	4	5/6	0.98	0.05	13,13,14,14	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	K	A	201	1/1	0.98	0.09	18,18,18,18	0
3	K	B	202	1/1	0.98	0.07	15,15,15,15	0
3	K	D	201	1/1	0.99	0.08	17,17,17,17	0
3	K	A	202	1/1	1.00	0.08	15,15,15,15	0
3	K	C	201	1/1	1.00	0.05	12,12,12,12	0
3	K	C	202	1/1	1.00	0.07	14,14,14,14	0
3	K	B	201	1/1	1.00	0.07	15,15,15,15	0
3	K	D	202	1/1	1.00	0.07	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.