



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:25 PM GMT

PDB ID : 4IAW  
Title : Engineered human lipocalin 2 (C26) in complex with Y-DTPA  
Authors : Eichinger, A.; Skerra, A.  
Deposited on : 2012-12-07  
Resolution : 2.40 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.

---

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

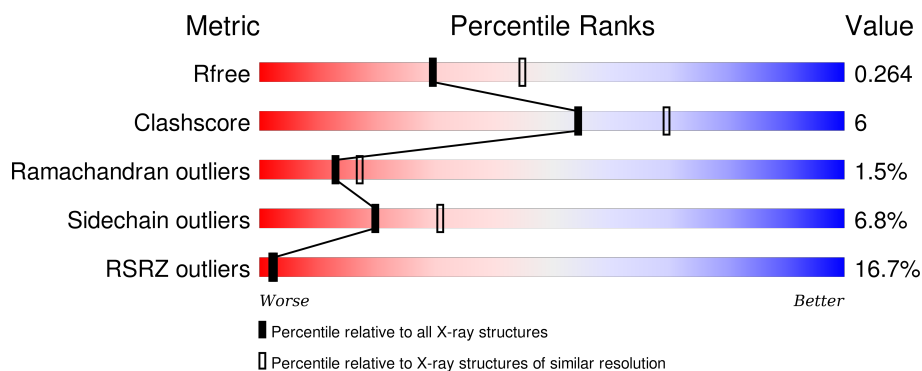
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


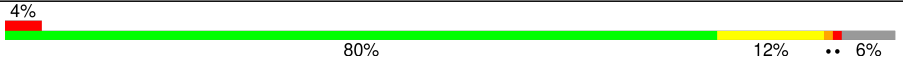

The reported resolution of this entry is 2.40 Å.

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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	188	
1	B	188	
1	C	188	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4536 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 Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1445	922	247	270	6			
1	B	176	Total	C	N	O	S	5	0	0
			1417	907	242	262	6			
1	C	172	Total	C	N	O	S	52	0	0
			1394	895	238	255	6			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	HIS	GLN	ENGINEERED MUTATION	UNP P80188
A	33	GLN	VAL	ENGINEERED MUTATION	UNP P80188
A	36	ARG	LEU	ENGINEERED MUTATION	UNP P80188
A	41	ALA	ILE	ENGINEERED MUTATION	UNP P80188
A	42	PRO	LEU	ENGINEERED MUTATION	UNP P80188
A	48	LEU	PRO	ENGINEERED MUTATION	UNP P80188
A	49	LEU	GLN	ENGINEERED MUTATION	UNP P80188
A	52	THR	TYR	ENGINEERED MUTATION	UNP P80188
A	54	GLN	THR	ENGINEERED MUTATION	UNP P80188
A	55	THR	ILE	ENGINEERED MUTATION	UNP P80188
A	68	ALA	SER	ENGINEERED MUTATION	UNP P80188
A	70	ARG	LEU	ENGINEERED MUTATION	UNP P80188
A	75	MET	LYS	ENGINEERED MUTATION	UNP P80188
A	77	GLU	ASP	ENGINEERED MUTATION	UNP P80188
A	79	LEU	TRP	ENGINEERED MUTATION	UNP P80188
A	80	THR	ILE	ENGINEERED MUTATION	UNP P80188
A	81	MET	ARG	ENGINEERED MUTATION	UNP P80188
A	87	SER	CYS	ENGINEERED MUTATION	UNP P80188
A	127	GLN	SER	ENGINEERED MUTATION	UNP P80188
A	134	SER	LYS	ENGINEERED MUTATION	UNP P80188
A	136	SER	THR	ENGINEERED MUTATION	UNP P80188
A	138	LEU	TYR	ENGINEERED MUTATION	UNP P80188
A	145	ALA	THR	ENGINEERED MUTATION	UNP P80188

*Continued on next page...*

*Continued from previous page...*

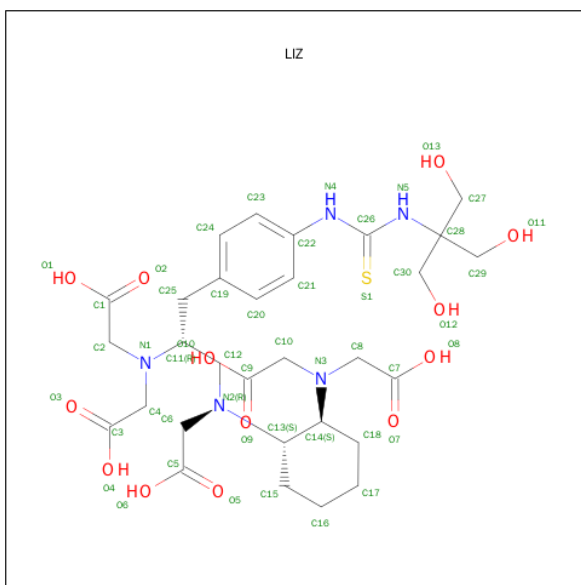
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	EXPRESSION TAG	UNP P80188
A	180	ALA	-	EXPRESSION TAG	UNP P80188
A	181	TRP	-	EXPRESSION TAG	UNP P80188
A	182	SER	-	EXPRESSION TAG	UNP P80188
A	183	HIS	-	EXPRESSION TAG	UNP P80188
A	184	PRO	-	EXPRESSION TAG	UNP P80188
A	185	GLN	-	EXPRESSION TAG	UNP P80188
A	186	PHE	-	EXPRESSION TAG	UNP P80188
A	187	GLU	-	EXPRESSION TAG	UNP P80188
A	188	LYS	-	EXPRESSION TAG	UNP P80188
B	28	HIS	GLN	ENGINEERED MUTATION	UNP P80188
B	33	GLN	VAL	ENGINEERED MUTATION	UNP P80188
B	36	ARG	LEU	ENGINEERED MUTATION	UNP P80188
B	41	ALA	ILE	ENGINEERED MUTATION	UNP P80188
B	42	PRO	LEU	ENGINEERED MUTATION	UNP P80188
B	48	LEU	PRO	ENGINEERED MUTATION	UNP P80188
B	49	LEU	GLN	ENGINEERED MUTATION	UNP P80188
B	52	THR	TYR	ENGINEERED MUTATION	UNP P80188
B	54	GLN	THR	ENGINEERED MUTATION	UNP P80188
B	55	THR	ILE	ENGINEERED MUTATION	UNP P80188
B	68	ALA	SER	ENGINEERED MUTATION	UNP P80188
B	70	ARG	LEU	ENGINEERED MUTATION	UNP P80188
B	75	MET	LYS	ENGINEERED MUTATION	UNP P80188
B	77	GLU	ASP	ENGINEERED MUTATION	UNP P80188
B	79	LEU	TRP	ENGINEERED MUTATION	UNP P80188
B	80	THR	ILE	ENGINEERED MUTATION	UNP P80188
B	81	MET	ARG	ENGINEERED MUTATION	UNP P80188
B	87	SER	CYS	ENGINEERED MUTATION	UNP P80188
B	127	GLN	SER	ENGINEERED MUTATION	UNP P80188
B	134	SER	LYS	ENGINEERED MUTATION	UNP P80188
B	136	SER	THR	ENGINEERED MUTATION	UNP P80188
B	138	LEU	TYR	ENGINEERED MUTATION	UNP P80188
B	145	ALA	THR	ENGINEERED MUTATION	UNP P80188
B	179	SER	-	EXPRESSION TAG	UNP P80188
B	180	ALA	-	EXPRESSION TAG	UNP P80188
B	181	TRP	-	EXPRESSION TAG	UNP P80188
B	182	SER	-	EXPRESSION TAG	UNP P80188
B	183	HIS	-	EXPRESSION TAG	UNP P80188
B	184	PRO	-	EXPRESSION TAG	UNP P80188
B	185	GLN	-	EXPRESSION TAG	UNP P80188
B	186	PHE	-	EXPRESSION TAG	UNP P80188
B	187	GLU	-	EXPRESSION TAG	UNP P80188

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	LYS	-	EXPRESSION TAG	UNP P80188
C	28	HIS	GLN	ENGINEERED MUTATION	UNP P80188
C	33	GLN	VAL	ENGINEERED MUTATION	UNP P80188
C	36	ARG	LEU	ENGINEERED MUTATION	UNP P80188
C	41	ALA	ILE	ENGINEERED MUTATION	UNP P80188
C	42	PRO	LEU	ENGINEERED MUTATION	UNP P80188
C	48	LEU	PRO	ENGINEERED MUTATION	UNP P80188
C	49	LEU	GLN	ENGINEERED MUTATION	UNP P80188
C	52	THR	TYR	ENGINEERED MUTATION	UNP P80188
C	54	GLN	THR	ENGINEERED MUTATION	UNP P80188
C	55	THR	ILE	ENGINEERED MUTATION	UNP P80188
C	68	ALA	SER	ENGINEERED MUTATION	UNP P80188
C	70	ARG	LEU	ENGINEERED MUTATION	UNP P80188
C	75	MET	LYS	ENGINEERED MUTATION	UNP P80188
C	77	GLU	ASP	ENGINEERED MUTATION	UNP P80188
C	79	LEU	TRP	ENGINEERED MUTATION	UNP P80188
C	80	THR	ILE	ENGINEERED MUTATION	UNP P80188
C	81	MET	ARG	ENGINEERED MUTATION	UNP P80188
C	87	SER	CYS	ENGINEERED MUTATION	UNP P80188
C	127	GLN	SER	ENGINEERED MUTATION	UNP P80188
C	134	SER	LYS	ENGINEERED MUTATION	UNP P80188
C	136	SER	THR	ENGINEERED MUTATION	UNP P80188
C	138	LEU	TYR	ENGINEERED MUTATION	UNP P80188
C	145	ALA	THR	ENGINEERED MUTATION	UNP P80188
C	179	SER	-	EXPRESSION TAG	UNP P80188
C	180	ALA	-	EXPRESSION TAG	UNP P80188
C	181	TRP	-	EXPRESSION TAG	UNP P80188
C	182	SER	-	EXPRESSION TAG	UNP P80188
C	183	HIS	-	EXPRESSION TAG	UNP P80188
C	184	PRO	-	EXPRESSION TAG	UNP P80188
C	185	GLN	-	EXPRESSION TAG	UNP P80188
C	186	PHE	-	EXPRESSION TAG	UNP P80188
C	187	GLU	-	EXPRESSION TAG	UNP P80188
C	188	LYS	-	EXPRESSION TAG	UNP P80188

- Molecule 2 is N-{(1S,2S)-2-[BIS(CARBOXYMETHYL)AMINO]CYCLOHEXYL}-N-{(2R)-2-[BIS(CARBOXYMETHYL)AMINO]-3-[4-({[2-HYDROXY-1,1-BIS(HYDROXYMETHYL)ETHYL]CARBAMOTHIOYL}AMINO)PHENYL]PROPYL}GLYCINE (three-letter code: LIZ) (formula: C<sub>30</sub>H<sub>45</sub>N<sub>5</sub>O<sub>13</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			42	26	5	10	1		
2	B	1	Total	C	N	O	S	0	0
			42	26	5	10	1		
2	C	1	Total	C	N	O	S	0	0
			42	26	5	10	1		

- Molecule 3 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Y	0	0
			1	1		
3	A	1	Total	Y	0	0
			1	1		
3	C	1	Total	Y	0	0
			1	1		

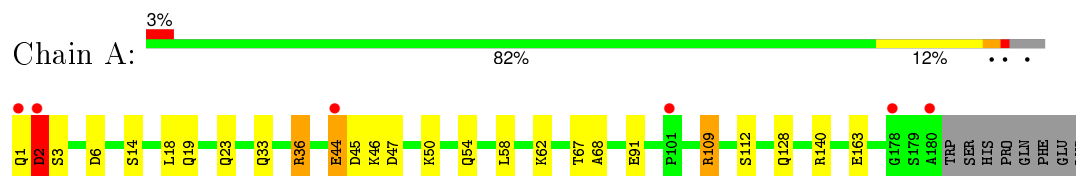
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	54	Total	O	0	0
			54	54		
4	C	4	Total	O	0	0
			4	4		

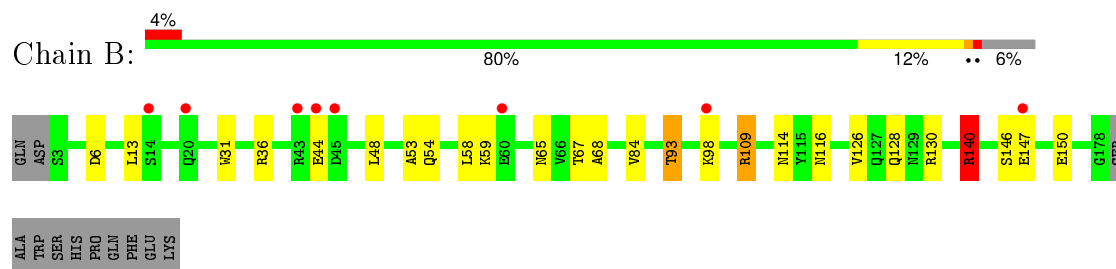
### 3 Residue-property plots [i](#)

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.

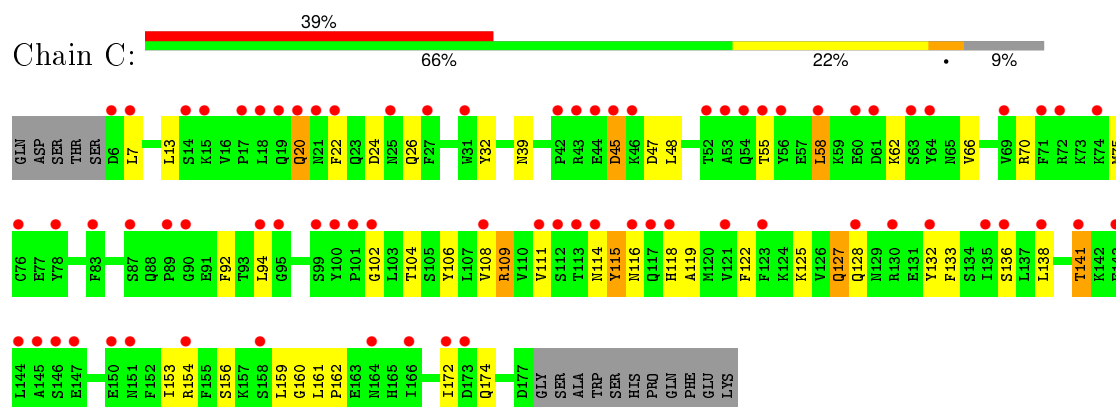
- Molecule 1: Neutrophil gelatinase-associated lipocalin



- Molecule 1: Neutrophil gelatinase-associated lipocalin



- Molecule 1: Neutrophil gelatinase-associated lipocalin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.26 Å   113.26 Å   119.98 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	82.36 – 2.40 19.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (82.36-2.40) 100.0 (19.94-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.52 (at 2.41 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.224   ,   0.270 0.215   ,   0.264	Depositor DCC
$R_{free}$ test set	1567 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31073 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: YT3, LIZ

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	0.82	0/1479	0.92	5/1999 (0.3%)
1	B	0.68	0/1451	0.76	1/1961 (0.1%)
1	C	0.47	0/1428	0.60	1/1930 (0.1%)
All	All	0.68	0/4358	0.77	7/5890 (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
1	A	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	A	140	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	A	36	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	C	58	LEU	CA-CB-CG	6.64	130.58	115.30
1	B	140	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	140	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	140	ARG	CG-CD-NE	-6.01	99.17	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ASP	Peptide

## 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	1445	0	1435	12	0
1	B	1417	0	1410	15	0
1	C	1394	0	1390	26	0
2	A	42	0	30	5	0
2	B	42	0	30	0	0
2	C	42	0	30	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	93	0	0	0	1
4	B	54	0	0	0	1
4	C	4	0	0	1	0
All	All	4536	0	4325	55	1

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 6.

All (55) 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:47:ASP:OD1	1:A:50:LYS:HE3	1.79	0.82
1:C:32:TYR:CD2	1:C:141:THR:O	2.35	0.80
1:A:23:GLN:NE2	1:B:140:ARG:HG2	2.02	0.73
1:C:109:ARG:HB3	1:C:122:PHE:HB3	1.70	0.73
1:B:84:VAL:HB	1:B:93:THR:HG22	1.73	0.69
1:C:39:ASN:HD21	1:C:132:TYR:HA	1.58	0.68
1:B:150:GLU:HG3	1:C:154:ARG:NH1	2.08	0.67
1:A:23:GLN:HE22	1:B:140:ARG:HG2	1.60	0.65
1:C:32:TYR:HD2	1:C:141:THR:O	1.79	0.64
1:C:92:PHE:HB2	1:C:108:VAL:HB	1.79	0.64
1:A:1:GLN:O	1:A:2:ASP:HB2	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ASN:HB3	1:C:133:PHE:CE1	2.38	0.58
1:A:33:GLN:OE1	1:A:36:ARG:HD3	2.03	0.58
1:C:20:GLN:NE2	4:C:302:HOH:O	2.34	0.56
1:A:91:GLU:OE1	1:A:109:ARG:NH1	2.34	0.56
1:C:125:LYS:HG3	1:C:132:TYR:HB2	1.91	0.53
1:C:114:ASN:C	1:C:116:ASN:H	2.12	0.53
1:B:59:LYS:HD3	1:B:65:ASN:ND2	2.24	0.52
1:C:26:GLN:O	1:C:115:TYR:HB3	2.08	0.52
1:B:31:TRP:CZ3	1:B:140:ARG:HD2	2.45	0.52
1:B:126:VAL:HA	1:B:130:ARG:O	2.10	0.51
1:C:22:PHE:HA	1:C:115:TYR:OH	2.11	0.50
1:C:119:ALA:HB3	1:C:138:LEU:HB2	1.92	0.50
1:C:153:ILE:HA	1:C:156:SER:HB2	1.93	0.49
1:B:36:ARG:NH2	1:B:48:LEU:O	2.38	0.49
2:A:201:LIZ:H21	2:A:201:LIZ:S1	2.52	0.49
1:C:156:SER:O	1:C:161:LEU:HB2	2.13	0.49
1:C:159:LEU:O	1:C:161:LEU:N	2.46	0.49
1:C:172:ILE:HD12	1:C:174:GLN:HB2	1.94	0.48
1:C:102:GLY:HA3	1:C:128:GLN:NE2	2.28	0.48
1:A:19:GLN:OE1	1:A:112:SER:HA	2.14	0.48
1:C:127:GLN:HG3	1:C:128:GLN:HG2	1.96	0.47
1:B:13:LEU:O	1:B:109:ARG:NH2	2.48	0.47
1:A:18:LEU:HD13	1:A:109:ARG:HD2	1.95	0.47
1:C:114:ASN:HB2	1:C:118:HIS:H	1.80	0.47
1:C:26:GLN:C	1:C:115:TYR:HB3	2.36	0.46
1:A:44:GLU:O	1:A:46:LYS:N	2.49	0.46
1:B:114:ASN:O	1:B:116:ASN:N	2.46	0.46
1:A:54:GLN:HA	1:A:67:THR:O	2.17	0.45
1:C:45:ASP:C	1:C:47:ASP:H	2.21	0.44
1:B:146:SER:O	1:B:150:GLU:HG2	2.18	0.44
1:B:54:GLN:HA	1:B:67:THR:O	2.18	0.43
1:C:94:LEU:HB2	1:C:106:TYR:CD1	2.53	0.43
1:A:68:ALA:HB3	2:A:201:LIZ:H15A	2.00	0.42
2:C:201:LIZ:H11	2:C:201:LIZ:O6	2.19	0.42
1:B:84:VAL:HB	1:B:93:THR:CG2	2.45	0.42
2:C:201:LIZ:H20	2:C:201:LIZ:H11	1.85	0.42
1:C:114:ASN:C	1:C:116:ASN:N	2.73	0.42
1:C:45:ASP:HB3	1:C:48:LEU:H	1.84	0.41
2:A:201:LIZ:S1	2:A:201:LIZ:C21	3.08	0.41
1:A:62:LYS:HD3	1:A:62:LYS:HA	1.83	0.41
2:A:201:LIZ:C5	2:A:201:LIZ:H11	2.50	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:LIZ:H25A	2:A:201:LIZ:H4	1.97	0.41
1:B:53:ALA:O	1:B:68:ALA:HA	2.21	0.41
1:B:150:GLU:HG3	1:C:154:ARG:HH11	1.81	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:392:HOH:O	4:B:354:HOH:O[8_554]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	178/188 (95%)	170 (96%)	6 (3%)	2 (1%)	17	25
1	B	174/188 (93%)	169 (97%)	5 (3%)	0	100	100
1	C	170/188 (90%)	146 (86%)	18 (11%)	6 (4%)	4	3
All	All	522/564 (93%)	485 (93%)	29 (6%)	8 (2%)	13	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	C	66	VAL
1	C	160	GLY
1	A	45	ASP
1	C	62	LYS
1	C	115	TYR
1	C	141	THR
1	C	162	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	161/169 (95%)	152 (94%)	9 (6%)	26	41
1	B	158/169 (94%)	149 (94%)	9 (6%)	25	40
1	C	155/169 (92%)	141 (91%)	14 (9%)	12	17
All	All	474/507 (94%)	442 (93%)	32 (7%)	20	31

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	SER
1	A	6	ASP
1	A	14	SER
1	A	44	GLU
1	A	58	LEU
1	A	109	ARG
1	A	128	GLN
1	A	163	GLU
1	B	6	ASP
1	B	44	GLU
1	B	58	LEU
1	B	93	THR
1	B	98	LYS
1	B	109	ARG
1	B	128	GLN
1	B	140	ARG
1	B	147	GLU
1	C	7	LEU
1	C	13	LEU
1	C	20	GLN
1	C	24	ASP
1	C	45	ASP
1	C	55	THR
1	C	58	LEU
1	C	70	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	75	MET
1	C	104	THR
1	C	109	ARG
1	C	111	VAL
1	C	127	GLN
1	C	136	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	128	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](#)

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, 3 are monoatomic - leaving 3 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$
2	LIZ	A	201	3	28,43,50	0.97	1 (3%)	36,58,68	1.91	7 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LIZ	B	201	3	28,43,50	0.86	0	36,58,68	2.01	8 (22%)
2	LIZ	C	201	3	28,43,50	0.88	1 (3%)	36,58,68	1.25	7 (19%)

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	LIZ	A	201	3	-	0/34/55/69	0/2/2/2
2	LIZ	B	201	3	-	0/34/55/69	0/2/2/2
2	LIZ	C	201	3	-	0/34/55/69	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	LIZ	C2-N1	-3.81	1.41	1.47
2	A	201	LIZ	C2-N1	-3.17	1.42	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	LIZ	S1-C26-N5	-7.08	113.58	123.18
2	B	201	LIZ	S1-C26-N5	-5.93	115.13	123.18
2	B	201	LIZ	C2-N1-C4	-4.73	104.86	110.88
2	B	201	LIZ	C6-N2-C13	-4.53	106.56	113.51
2	A	201	LIZ	C2-N1-C4	-4.16	105.58	110.88
2	A	201	LIZ	C10-N3-C14	-4.00	107.38	113.51
2	B	201	LIZ	C10-N3-C14	-3.62	107.95	113.51
2	C	201	LIZ	C10-N3-C14	-3.51	108.13	113.51
2	C	201	LIZ	C2-N1-C4	-2.97	107.09	110.88
2	A	201	LIZ	C10-N3-C8	-2.67	107.47	110.88
2	B	201	LIZ	C10-N3-C8	-2.53	107.65	110.88
2	C	201	LIZ	C10-N3-C8	-2.45	107.75	110.88
2	C	201	LIZ	C2-N1-C11	-2.30	108.05	113.01
2	C	201	LIZ	S1-C26-N5	-2.24	120.14	123.18
2	C	201	LIZ	C12-N2-C13	-2.04	108.38	112.93
2	C	201	LIZ	C22-N4-C26	-2.03	122.66	128.56
2	B	201	LIZ	C22-N4-C26	2.03	134.48	128.56
2	A	201	LIZ	C16-C15-C13	2.07	115.41	110.38
2	A	201	LIZ	S1-C26-N4	2.43	124.14	120.77
2	B	201	LIZ	C2-N1-C11	2.55	118.52	113.01

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	LIZ	N5-C26-N4	3.88	122.29	117.97
2	B	201	LIZ	S1-C26-N4	4.93	127.59	120.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	LIZ	5	0
2	C	201	LIZ	2	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	180/188 (95%)	-0.07	6 (3%)	50 50	6, 20, 44, 56	0
1	B	176/188 (93%)	0.03	8 (4%)	37 38	16, 29, 44, 62	1 (0%)
1	C	172/188 (91%)	1.93	74 (43%)	0 0	65, 81, 94, 96	12 (6%)
All	All	528/564 (93%)	0.61	88 (16%)	2 2	6, 33, 93, 96	13 (2%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	LEU	9.6
1	C	147	GLU	6.6
1	A	2	ASP	5.4
1	C	164	ASN	5.3
1	C	154	ARG	4.9
1	C	121	VAL	4.8
1	C	45	ASP	4.8
1	C	43	ARG	4.7
1	C	18	LEU	4.6
1	C	6	ASP	4.3
1	C	118	HIS	4.2
1	C	116	ASN	4.0
1	C	60	GLU	4.0
1	C	158	SER	3.9
1	C	146	SER	3.7
1	C	101	PRO	3.7
1	C	27	PHE	3.6
1	C	95	GLY	3.6
1	B	98	LYS	3.5
1	C	17	PRO	3.5
1	C	114	ASN	3.5
1	A	1	GLN	3.5
1	C	132	TYR	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	44	GLU	3.4
1	C	14	SER	3.3
1	C	21	ASN	3.3
1	C	44	GLU	3.2
1	C	150	GLU	3.2
1	C	151	ASN	3.2
1	C	99	SER	3.2
1	C	56	TYR	3.2
1	A	44	GLU	3.2
1	C	46	LYS	3.1
1	C	102	GLY	3.1
1	C	78	TYR	3.1
1	C	76	CYS	3.1
1	C	64	TYR	3.1
1	C	143	GLU	3.1
1	C	69	VAL	3.1
1	C	112	SER	3.1
1	C	53	ALA	3.0
1	C	113	THR	3.0
1	C	20	GLN	3.0
1	C	94	LEU	3.0
1	C	63	SER	3.0
1	C	54	GLN	2.9
1	C	144	LEU	2.9
1	C	136	SER	2.9
1	C	89	PRO	2.8
1	C	111	VAL	2.8
1	C	130	ARG	2.8
1	B	20	GLN	2.7
1	C	138	LEU	2.7
1	B	147	GLU	2.7
1	C	22	PHE	2.7
1	C	72	ARG	2.7
1	C	172	ILE	2.6
1	C	173	ASP	2.6
1	A	178	GLY	2.6
1	C	135	ILE	2.5
1	C	15	LYS	2.5
1	C	52	THR	2.5
1	C	141	THR	2.5
1	C	128	GLN	2.5
1	C	74	LYS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	117	GLN	2.5
1	C	123	PHE	2.4
1	C	108	VAL	2.4
1	C	166	ILE	2.4
1	B	43	ARG	2.4
1	C	87	SER	2.4
1	C	7	LEU	2.3
1	C	55	THR	2.3
1	C	71	PHE	2.3
1	C	100	TYR	2.3
1	C	25	ASN	2.3
1	C	31	TRP	2.3
1	C	61	ASP	2.2
1	C	19	GLN	2.2
1	C	83	PHE	2.1
1	B	45	ASP	2.1
1	C	42	PRO	2.1
1	B	14	SER	2.1
1	A	180	ALA	2.0
1	C	145	ALA	2.0
1	A	101	PRO	2.0
1	B	60	GLU	2.0
1	C	90	GLY	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
2	LIZ	C	201	42/49	0.84	0.22	-0.69	60,70,83,87	0
2	LIZ	A	201	42/49	0.96	0.13	-0.69	9,16,35,50	0
2	LIZ	B	201	42/49	0.95	0.12	-0.98	9,18,41,57	0
3	YT3	A	202	1/1	1.00	0.07	-	14,14,14,14	0
3	YT3	B	202	1/1	1.00	0.07	-	19,19,19,19	0
3	YT3	C	202	1/1	0.98	0.06	-	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.