



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 09:11 pm GMT

PDB ID : 2WS6  
Title : Semi-synthetic analogue of human insulin NMeTyrB26-insulin in hexamer form  
Authors : Brzozowski, A.M.; Jiracek, J.; Zakova, L.; Antolikova, E.; Watson, C.J.;  
Turkenburg, J.P.; Dodson, G.G.  
Deposited on : 2009-09-03  
Resolution : 1.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

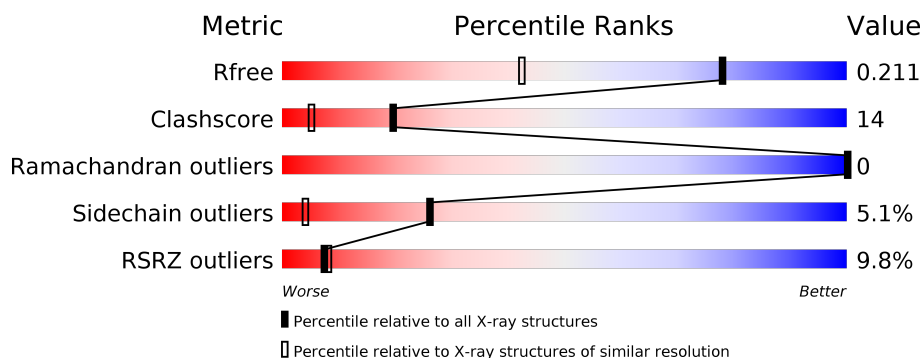
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	111664	2534 (1.50-1.50)
Clashscore	122126	2727 (1.50-1.50)
Ramachandran outliers	120053	2661 (1.50-1.50)
Sidechain outliers	120020	2659 (1.50-1.50)
RSRZ outliers	108989	2481 (1.50-1.50)

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	21	<div> <div>33%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div>
1	C	21	<div> <div>10%</div> <div> <div></div> <div>71%</div> <div>29%</div> </div> </div>
1	E	21	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>10%</div> </div> </div>
1	G	21	<div> <div></div> <div> <div></div> <div>76%</div> <div>24%</div> </div> </div>
1	I	21	<div> <div></div> <div> <div></div> <div>71%</div> <div>19%</div> <div>5%</div> <div>5%</div> </div> </div>
1	K	21	<div> <div>14%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	30	<div> <div>3%</div> <div>57%</div> <div>30%</div> <div>13%</div> </div>
2	D	30	<div> <div>17%</div> <div>57%</div> <div>27%</div> <div>7%</div> <div>10%</div> </div>
3	F	30	<div> <div>17%</div> <div>77%</div> <div>20%</div> <div>•</div> </div>
3	H	30	<div> <div>7%</div> <div>63%</div> <div>23%</div> <div>•</div> <div>10%</div> </div>
3	J	30	<div> <div>7%</div> <div>70%</div> <div>20%</div> <div>•</div> <div>7%</div> </div>
3	L	30	<div> <div>67%</div> <div>20%</div> <div>•</div> <div>10%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2773 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 INSULIN A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	6	1	0
			171	103	27	37	4			
1	C	21	Total	C	N	O	S	4	0	0
			163	99	25	35	4			
1	E	21	Total	C	N	O	S	0	1	0
			171	105	26	36	4			
1	G	21	Total	C	N	O	S	0	1	0
			172	104	27	37	4			
1	I	21	Total	C	N	O	S	10	2	0
			181	109	28	40	4			
1	K	21	Total	C	N	O	S	4	3	0
			189	113	30	42	4			

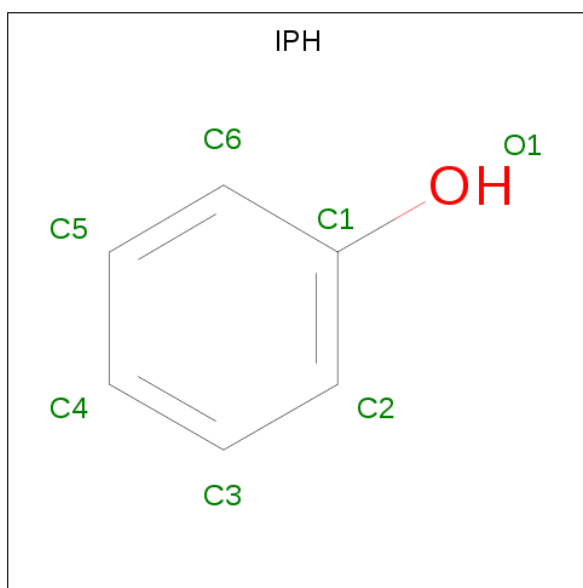
- Molecule 2 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	26	Total	C	N	O	S	4	2	0
			229	149	38	40	2			
2	D	27	Total	C	N	O	S	6	2	0
			238	154	41	41	2			

- Molecule 3 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	29	Total	C	N	O	S	5	2	0
			254	167	44	41	2			
3	H	27	Total	C	N	O	S	3	4	0
			253	164	44	43	2			
3	J	28	Total	C	N	O	S	0	0	0
			226	149	37	38	2			
3	L	27	Total	C	N	O	S	6	1	0
			230	150	40	38	2			

- Molecule 4 is PHENOL (three-letter code: IPH) (formula:  $C_6H_6O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	6	1		
4	C	1	Total	C	O	0	0
			7	6	1		
4	E	1	Total	C	O	0	0
			7	6	1		
4	G	1	Total	C	O	0	0
			7	6	1		
4	I	1	Total	C	O	0	0
			7	6	1		
4	K	1	Total	C	O	0	0
			7	6	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Cl	0	0
			1	1		
5	L	1	Total	Cl	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	1	Total	Zn	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total	O	0	0
			8	8		
8	B	26	Total	O	0	0
			26	26		
8	C	24	Total	O	0	0
			24	24		
8	D	17	Total	O	0	0
			17	17		
8	E	12	Total	O	0	0
			12	12		
8	F	19	Total	O	0	0
			19	19		
8	G	20	Total	O	0	0
			20	20		

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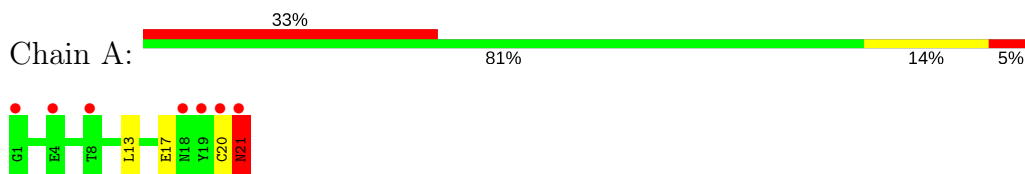
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	26	Total 26	O 26	0	0
8	I	24	Total 24	O 24	0	0
8	J	26	Total 26	O 26	0	0
8	K	16	Total 16	O 16	0	0
8	L	26	Total 26	O 26	0	0

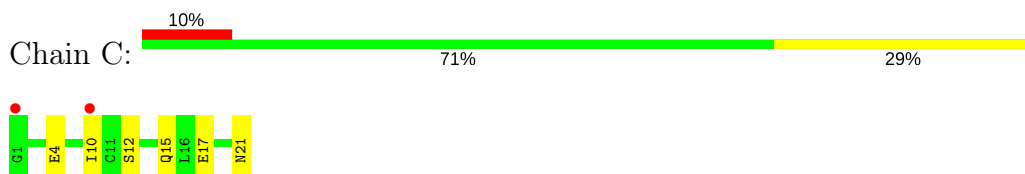
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: INSULIN A CHAIN



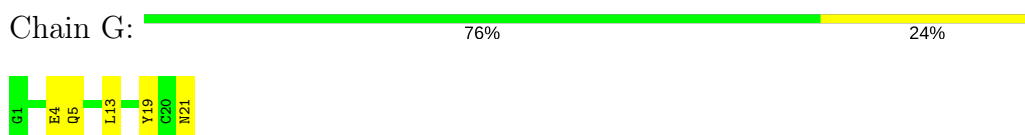
- Molecule 1: INSULIN A CHAIN



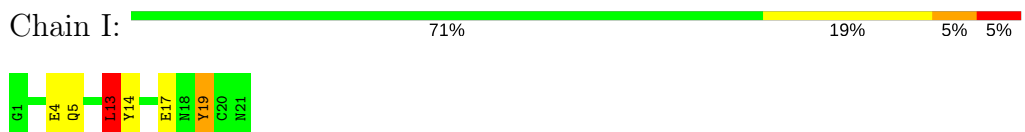
- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN



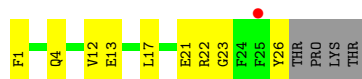
- Molecule 1: INSULIN A CHAIN







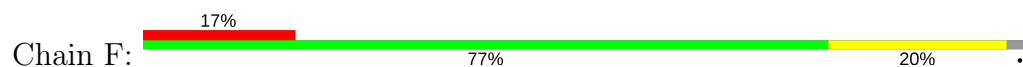
• Molecule 2: INSULIN B CHAIN



• Molecule 2: INSULIN B CHAIN



• Molecule 3: INSULIN B CHAIN



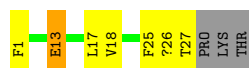
• Molecule 3: INSULIN B CHAIN



• Molecule 3: INSULIN B CHAIN



• Molecule 3: INSULIN B CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.96Å 61.93Å 47.30Å 90.00° 111.90° 90.00°	Depositor
Resolution (Å)	40.00 – 1.50 35.81 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.50) 99.7 (35.81-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0082	Depositor
R, $R_{free}$	0.150 , 0.200 0.165 , 0.211	Depositor DCC
$R_{free}$ test set	2565 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h-l,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YNM, ZN, CL, IPH, GOL

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	1.04	0/172	1.08	1/231 (0.4%)
1	C	1.46	3/164 (1.8%)	1.04	0/220
1	E	1.54	2/172 (1.2%)	0.90	0/231
1	G	1.42	1/173 (0.6%)	0.87	0/232
1	I	1.33	2/182 (1.1%)	1.09	1/244 (0.4%)
1	K	1.19	0/190	0.91	0/255
2	B	1.39	2/235 (0.9%)	0.97	0/316
2	D	1.54	4/244 (1.6%)	1.29	0/328
3	F	1.28	1/246 (0.4%)	1.05	0/329
3	H	1.26	2/244 (0.8%)	0.88	0/326
3	J	1.48	2/218 (0.9%)	1.04	1/293 (0.3%)
3	L	1.76	4/221 (1.8%)	1.53	5/295 (1.7%)
All	All	1.41	23/2461 (0.9%)	1.08	8/3300 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	D	1	0
All	All	1	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	13	GLU	CB-CG	-13.49	1.26	1.52
3	L	1	PHE	CB-CG	-9.42	1.35	1.51
2	B	21	GLU	CB-CG	-7.80	1.37	1.52
1	C	4	GLU	CB-CG	-7.78	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	7	CYS	CB-SG	-7.61	1.69	1.82
2	D	13[A]	GLU	CD-OE2	7.40	1.33	1.25
2	D	13[B]	GLU	CD-OE2	7.40	1.33	1.25
1	C	17	GLU	CB-CG	-7.05	1.38	1.52
1	I	4	GLU	CG-CD	-6.44	1.42	1.51
1	G	19	TYR	CD2-CE2	-6.36	1.29	1.39
2	D	13[A]	GLU	CG-CD	5.89	1.60	1.51
2	D	13[B]	GLU	CG-CD	5.89	1.60	1.51
3	H	21	GLU	CG-CD	5.78	1.60	1.51
1	E	14	TYR	CE2-CZ	-5.50	1.31	1.38
3	J	16	TYR	CD1-CE1	-5.46	1.31	1.39
3	L	13	GLU	CD-OE2	5.43	1.31	1.25
2	B	12	VAL	CB-CG2	5.36	1.64	1.52
3	H	13	GLU	CD-OE2	5.26	1.31	1.25
1	C	17	GLU	CD-OE1	5.21	1.31	1.25
3	L	18	VAL	CB-CG1	-5.19	1.42	1.52
3	F	21	GLU	CB-CG	-5.17	1.42	1.52
1	I	19	TYR	CE1-CZ	-5.08	1.31	1.38
3	J	21	GLU	CB-CG	-5.00	1.42	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	PHE	CB-CG-CD2	10.66	128.26	120.80
3	L	1	PHE	CB-CG-CD1	-10.62	113.37	120.80
1	I	13	LEU	CB-CG-CD1	-7.30	98.60	111.00
3	L	13	GLU	CG-CD-OE1	-6.89	104.52	118.30
3	L	13	GLU	CB-CG-CD	-6.29	97.23	114.20
3	L	1	PHE	CA-CB-CG	6.09	128.51	113.90
3	J	22	ARG	CG-CD-NE	5.62	123.59	111.80
1	A	21	ASN	CB-CA-C	-5.18	100.03	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	27	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	CYS	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	171	0	154	8	0
1	C	163	0	149	5	0
1	E	171	0	159	7	0
1	G	172	0	156	3	0
1	I	181	0	161	6	0
1	K	189	0	167	7	0
2	B	229	0	210	13	0
2	D	238	0	222	11	0
3	F	254	0	249	14	0
3	H	253	0	240	11	0
3	J	226	0	214	5	1
3	L	230	0	219	8	0
4	A	7	0	5	0	0
4	C	7	0	5	0	0
4	E	7	0	5	0	0
4	G	7	0	5	0	0
4	I	7	0	5	0	0
4	K	7	0	6	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
7	L	6	0	8	3	0
8	A	8	0	0	0	0
8	B	26	0	0	6	0
8	C	24	0	0	2	1
8	D	17	0	0	0	0
8	E	12	0	0	1	0
8	F	19	0	0	2	0
8	G	20	0	0	0	0
8	H	26	0	0	1	0
8	I	24	0	0	0	0
8	J	26	0	0	1	0
8	K	16	0	0	3	0
8	L	26	0	0	3	0
All	All	2773	0	2339	66	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 14.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:17[B]:LEU:CD2	1:K:13:LEU:HD21	1.51	1.38
3:F:17[B]:LEU:HD21	1:K:13:LEU:CD2	1.69	1.23
8:F:2008:HOH:O	3:H:13:GLU:HG2	1.10	1.21
3:H:17[A]:LEU:HD21	8:H:2008:HOH:O	1.03	1.19
2:B:13[A]:GLU:HG3	8:B:2012:HOH:O	1.57	1.04
2:B:13[A]:GLU:HG2	8:B:2017:HOH:O	1.55	1.02
2:B:26:TYR:C	8:B:2025:HOH:O	2.07	0.94
1:A:13:LEU:HD21	3:H:17[B]:LEU:HG	1.57	0.86
1:A:13:LEU:HD21	3:H:17[B]:LEU:CG	2.06	0.85
2:B:13[B]:GLU:OE1	2:D:9:SER:OG	1.96	0.84
1:A:21:ASN:HA	2:B:23:GLY:O	1.78	0.83
2:B:13[A]:GLU:CG	8:B:2012:HOH:O	2.22	0.79
2:B:17:LEU:HD23	3:H:17[B]:LEU:HD23	1.65	0.76
1:E:5:GLN:O	8:E:2001:HOH:O	2.06	0.74
3:L:13:GLU:CD	8:L:2011:HOH:O	2.26	0.73
8:J:2006:HOH:O	3:L:13:GLU:HG2	1.89	0.72
3:F:17[B]:LEU:HD21	1:K:13:LEU:HD21	0.78	0.72
1:C:21:ASN:O	2:D:22[B]:ARG:HD2	1.90	0.72
3:F:17[B]:LEU:CD1	8:K:2012:HOH:O	2.38	0.71
3:F:17[B]:LEU:CD2	1:K:13:LEU:CD2	2.47	0.70
1:C:21:ASN:O	2:D:22[A]:ARG:HD3	1.92	0.69
3:L:27:THR:H	7:L:1030:GOL:C1	2.04	0.69
3:F:17[B]:LEU:CG	1:K:13:LEU:HD21	2.25	0.64
3:F:17[B]:LEU:HD23	3:L:17:LEU:HD23	1.80	0.63
3:L:13:GLU:HG3	8:L:2010:HOH:O	1.98	0.63
1:C:21:ASN:OXT	8:C:2024:HOH:O	2.16	0.63
1:I:5[B]:GLN:NE2	1:I:19:TYR:OH	2.31	0.62
2:D:17:LEU:HG	1:I:13:LEU:HD21	1.81	0.62
1:A:13:LEU:HD21	3:H:17[B]:LEU:CD1	2.30	0.61
3:F:23:GLY:HA3	3:H:27:THR:HG22	1.82	0.61
8:B:2020:HOH:O	2:D:5:HIS:HD2	1.84	0.60
3:F:17[B]:LEU:HD11	8:K:2012:HOH:O	2.01	0.60
1:I:17[B]:GLU:HG2	3:J:18:VAL:CG1	2.33	0.59
1:E:10[B]:ILE:HG12	3:J:2:VAL:HG22	1.84	0.59
1:A:17:GLU:OE2	2:B:22:ARG:NH1	2.36	0.58
3:L:27:THR:H	7:L:1030:GOL:H11	1.69	0.57
1:E:2:ILE:HG22	8:F:2017:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:17[B]:LEU:HG	1:K:13:LEU:HG	1.88	0.56
1:A:13:LEU:HD21	3:H:17[B]:LEU:HD11	1.88	0.56
1:C:12:SER:H	1:C:15:GLN:HE21	1.54	0.55
2:D:13[A]:GLU:HG2	3:J:13:GLU:OE1	2.07	0.54
2:D:19:CYS:O	2:D:22[B]:ARG:HG2	2.09	0.53
1:E:3:VAL:O	1:E:7:CYS:HB2	2.10	0.52
1:C:12:SER:H	1:C:15:GLN:NE2	2.10	0.50
2:B:1:PHE:O	2:B:4[B]:GLN:HG3	2.13	0.48
2:B:17:LEU:HG	1:G:13:LEU:HD21	1.95	0.48
3:F:17[B]:LEU:HG	1:K:13:LEU:CG	2.44	0.47
2:D:13[A]:GLU:CG	3:J:13:GLU:OE1	2.62	0.47
3:H:25:PHE:HA	3:H:26:YNM:HM1C	1.64	0.47
1:A:21:ASN:ND2	2:B:22:ARG:HE	2.13	0.46
1:E:4:GLU:O	1:E:8:THR:HG23	2.15	0.46
2:D:17:LEU:HG	1:I:13:LEU:CD2	2.44	0.46
2:D:3:ASN:HB2	8:L:2002:HOH:O	2.15	0.46
1:A:21:ASN:HD22	2:B:22:ARG:HB3	1.81	0.45
1:E:2:ILE:HD13	1:E:19:TYR:CE2	2.52	0.45
1:I:13:LEU:HA	1:I:13:LEU:HD22	1.82	0.45
3:L:26:YNM:HA	7:L:1030:GOL:H12	1.99	0.45
8:C:2024:HOH:O	2:D:22[A]:ARG:NH1	2.50	0.44
1:E:2:ILE:O	1:E:2:ILE:HD12	2.18	0.44
2:B:4[B]:GLN:NE2	8:B:2007:HOH:O	2.41	0.44
3:L:25:PHE:HA	3:L:26:YNM:HM1C	1.69	0.43
1:I:13:LEU:HD11	3:J:18:VAL:HG22	2.01	0.43
3:F:17[B]:LEU:HD12	8:K:2012:HOH:O	2.10	0.42
3:F:13:GLU:OE2	3:H:9[B]:SER:OG	2.35	0.41
3:F:27:THR:HG22	1:G:21:ASN:ND2	2.36	0.40
1:G:21:ASN:HB2	3:H:22[A]:ARG:O	2.21	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)
3:J:1:PHE:CB	8:C:2023:HOH:O[2_645]	2.11	0.09

## 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	20/21 (95%)	20 (100%)	0	0	100	100
1	C	19/21 (90%)	19 (100%)	0	0	100	100
1	E	20/21 (95%)	20 (100%)	0	0	100	100
1	G	20/21 (95%)	20 (100%)	0	0	100	100
1	I	21/21 (100%)	21 (100%)	0	0	100	100
1	K	22/21 (105%)	22 (100%)	0	0	100	100
2	B	26/30 (87%)	26 (100%)	0	0	100	100
2	D	27/30 (90%)	27 (100%)	0	0	100	100
3	F	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
3	H	28/30 (93%)	28 (100%)	0	0	100	100
3	J	25/30 (83%)	25 (100%)	0	0	100	100
3	L	25/30 (83%)	25 (100%)	0	0	100	100
All	All	281/306 (92%)	279 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	21/20 (105%)	20 (95%)	1 (5%)	28	4
1	C	20/20 (100%)	19 (95%)	1 (5%)	27	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	21/20 (105%)	20 (95%)	1 (5%)	28	4
1	G	21/20 (105%)	19 (90%)	2 (10%)	9	0
1	I	22/20 (110%)	20 (91%)	2 (9%)	10	0
1	K	23/20 (115%)	23 (100%)	0	100	100
2	B	24/26 (92%)	24 (100%)	0	100	100
2	D	25/26 (96%)	21 (84%)	4 (16%)	2	0
3	F	26/25 (104%)	25 (96%)	1 (4%)	36	8
3	H	26/25 (104%)	26 (100%)	0	100	100
3	J	23/25 (92%)	22 (96%)	1 (4%)	32	6
3	L	23/25 (92%)	23 (100%)	0	100	100
All	All	275/272 (101%)	262 (95%)	13 (5%)	26	5

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	C	10	ILE
2	D	1	PHE
2	D	2	VAL
2	D	3	ASN
2	D	27	THR
1	E	2	ILE
3	F	25	PHE
1	G	4	GLU
1	G	5	GLN
1	I	13	LEU
1	I	14	TYR
3	J	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	21	ASN
1	C	15	GLN
2	D	5	HIS
1	E	21	ASN

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Mol	Chain	Res	Type
3	F	3	ASN
3	F	5	HIS
3	J	3	ASN
3	J	4	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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$
3	YNM	F	26	3	13,13,14	1.55	2 (15%)	15,16,18	1.10	1 (6%)
3	YNM	H	26	3	13,13,14	1.38	1 (7%)	15,16,18	1.13	2 (13%)
3	YNM	J	26	3	13,13,14	1.30	2 (15%)	15,16,18	1.27	1 (6%)
3	YNM	L	26	3	13,13,14	1.58	2 (15%)	15,16,18	1.08	1 (6%)

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	YNM	F	26	3	-	0/4/8/10	0/1/1/1
3	YNM	H	26	3	-	0/4/8/10	0/1/1/1
3	YNM	J	26	3	-	0/4/8/10	0/1/1/1
3	YNM	L	26	3	-	0/4/8/10	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	26	YNM	CE2-CD2	-3.81	1.32	1.38
3	J	26	YNM	CA-C	2.26	1.53	1.50
3	J	26	YNM	OH-CZ	2.40	1.42	1.37
3	F	26	YNM	CA-C	2.48	1.53	1.50
3	L	26	YNM	O-C	2.69	1.30	1.19
3	H	26	YNM	CA-C	2.79	1.53	1.50
3	L	26	YNM	CA-C	3.67	1.55	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	26	YNM	CG-CB-CA	-4.20	107.74	113.71
3	L	26	YNM	CG-CB-CA	-3.14	109.25	113.71
3	H	26	YNM	CG-CB-CA	-2.98	109.47	113.71
3	F	26	YNM	CD1-CE1-CZ	-2.83	116.73	119.88
3	H	26	YNM	CM-N-CA	2.14	120.59	113.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	26	YNM	1	0
3	L	26	YNM	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
4	IPH	A	1022	-	7,7,7	0.92	0	8,8,8	0.61	0
4	IPH	C	1022	-	7,7,7	0.74	0	8,8,8	1.32	2 (25%)
4	IPH	E	1022	-	7,7,7	1.23	0	8,8,8	0.70	0
4	IPH	G	1022	-	7,7,7	0.95	0	8,8,8	0.90	0
4	IPH	I	1022	-	7,7,7	1.09	0	8,8,8	0.57	0
4	IPH	K	1022	-	7,7,7	1.03	1 (14%)	8,8,8	1.42	2 (25%)
7	GOL	L	1030	-	5,5,5	0.41	0	5,5,5	1.58	1 (20%)

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	IPH	A	1022	-	-	0/0/0/0	0/1/1/1
4	IPH	C	1022	-	-	0/0/0/0	0/1/1/1
4	IPH	E	1022	-	-	0/0/0/0	0/1/1/1
4	IPH	G	1022	-	-	0/0/0/0	0/1/1/1
4	IPH	I	1022	-	-	0/0/0/0	0/1/1/1
4	IPH	K	1022	-	-	0/0/0/0	0/1/1/1
7	GOL	L	1030	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1022	IPH	C6-C1	-2.05	1.34	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1022	IPH	C4-C5-C6	-2.41	116.89	120.20
4	K	1022	IPH	C6-C1-C2	-2.07	116.11	119.75
4	C	1022	IPH	C5-C6-C1	2.35	122.87	119.36
4	K	1022	IPH	C5-C6-C1	2.55	123.16	119.36
7	L	1030	GOL	O2-C2-C3	3.09	123.13	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1030	GOL	3	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	21/21 (100%)	1.57	7 (33%) 0 0	16, 21, 28, 34	1 (4%)
1	C	21/21 (100%)	0.27	2 (9%) 8 9	11, 19, 31, 32	1 (4%)
1	E	21/21 (100%)	0.12	1 (4%) 30 33	11, 21, 29, 34	0
1	G	21/21 (100%)	0.13	0 100 100	12, 18, 29, 38	0
1	I	21/21 (100%)	-0.17	0 100 100	11, 15, 19, 23	2 (9%)
1	K	21/21 (100%)	0.71	3 (14%) 2 2	12, 17, 23, 25	1 (4%)
2	B	26/30 (86%)	0.41	1 (3%) 40 45	8, 14, 28, 35	1 (3%)
2	D	27/30 (90%)	1.09	5 (18%) 1 1	10, 15, 31, 41	1 (3%)
3	F	28/30 (93%)	0.99	5 (17%) 1 1	10, 14, 28, 36	1 (3%)
3	H	26/30 (86%)	0.58	2 (7%) 13 14	10, 13, 21, 27	1 (3%)
3	J	27/30 (90%)	0.63	2 (7%) 14 15	10, 14, 27, 29	0
3	L	26/30 (86%)	0.33	0 100 100	9, 13, 22, 26	1 (3%)
All	All	286/306 (93%)	0.57	28 (9%) 7 8	8, 16, 30, 41	10 (3%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	25	PHE	8.6
2	D	1	PHE	8.3
3	F	1	PHE	6.4
2	D	25	PHE	5.5
1	A	1	GLY	5.1
1	K	14	TYR	4.9
1	A	18[A]	ASN	4.0
1	A	21	ASN	3.4
2	D	26	TYR	3.3
1	C	10	ILE	3.2
1	E	9	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	J	1	PHE	3.1
2	D	27	THR	2.9
1	K	18[A]	ASN	2.9
1	C	1	GLY	2.8
1	A	4	GLU	2.7
3	F	25	PHE	2.6
3	F	29	LYS	2.6
2	D	2	VAL	2.5
3	J	12	VAL	2.4
1	K	1	GLY	2.4
1	A	19	TYR	2.4
1	A	8	THR	2.3
3	F	17[A]	LEU	2.2
3	H	11	LEU	2.2
3	F	22[A]	ARG	2.1
3	H	12	VAL	2.1
1	A	20	CYS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	YNM	F	26	13/14	0.95	0.08	15,16,26,28	0
3	YNM	H	26	13/14	0.95	0.08	14,15,19,23	0
3	YNM	L	26	13/14	0.96	0.07	14,16,19,22	0
3	YNM	J	26	13/14	0.97	0.08	12,12,15,17	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 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. 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( $\text{\AA}^2$ )	Q<0.9
7	GOL	L	1030	6/6	0.89	0.19	24,30,35,39	0
4	IPH	E	1022	7/7	0.95	0.09	15,16,18,23	0
4	IPH	C	1022	7/7	0.96	0.11	16,18,20,21	0
4	IPH	A	1022	7/7	0.96	0.10	14,16,17,17	0
4	IPH	G	1022	7/7	0.96	0.13	15,15,17,17	0
4	IPH	I	1022	7/7	0.97	0.12	12,12,14,15	0
4	IPH	K	1022	7/7	0.97	0.12	11,12,13,15	0
5	CL	L	1028	1/1	1.00	0.09	11,11,11,11	0
5	CL	J	1029	1/1	1.00	0.11	10,10,10,10	0
6	ZN	L	1029	1/1	1.00	0.12	10,10,10,10	0
6	ZN	J	1030	1/1	1.00	0.13	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.