



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 11:00 pm GMT

PDB ID : 2WC0
Title : crystal structure of human insulin degrading enzyme in complex with iodinated insulin
Authors : Manolopoulou, M.; Guo, Q.; Malito, E.; Schilling, A.B.; Tang, W.J.
Deposited on : 2009-03-06
Resolution : 2.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
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)	:	trunk30967

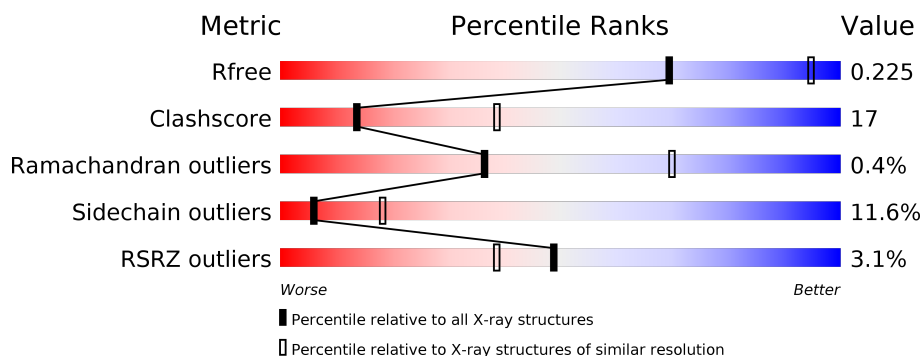
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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 ≥ 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	990	
1	B	990	
2	C	21	
2	E	21	
3	D	30	
3	F	30	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16597 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-DEGRADING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	1
			7781	5013	1307	1439	22			
1	B	955	Total	C	N	O	S	0	0	1
			7790	5019	1308	1441	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called INSULIN A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total 155	C 95	N 24	O 32	S 4	0	0	1
2	E	21	Total 155	C 95	N 24	O 32	S 4	0	0	1

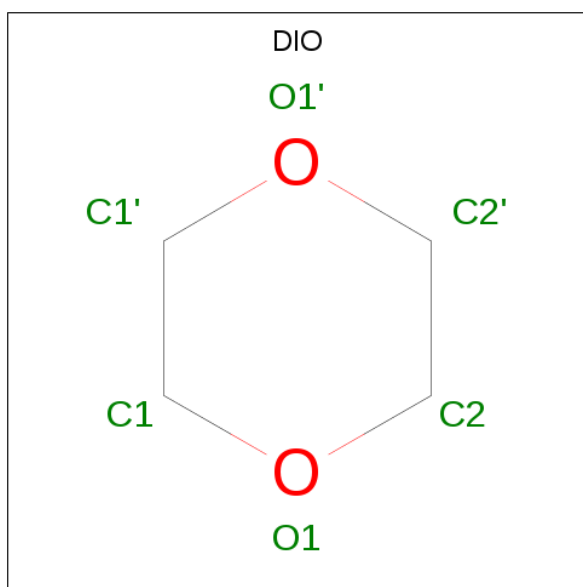
- Molecule 3 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total 153	C 99	N 26	O 26	S 2	0	0	0
3	F	20	Total 153	C 99	N 26	O 26	S 2	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total	O	0	0
			189	189		
6	B	163	Total	O	0	0
			163	163		
6	C	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		

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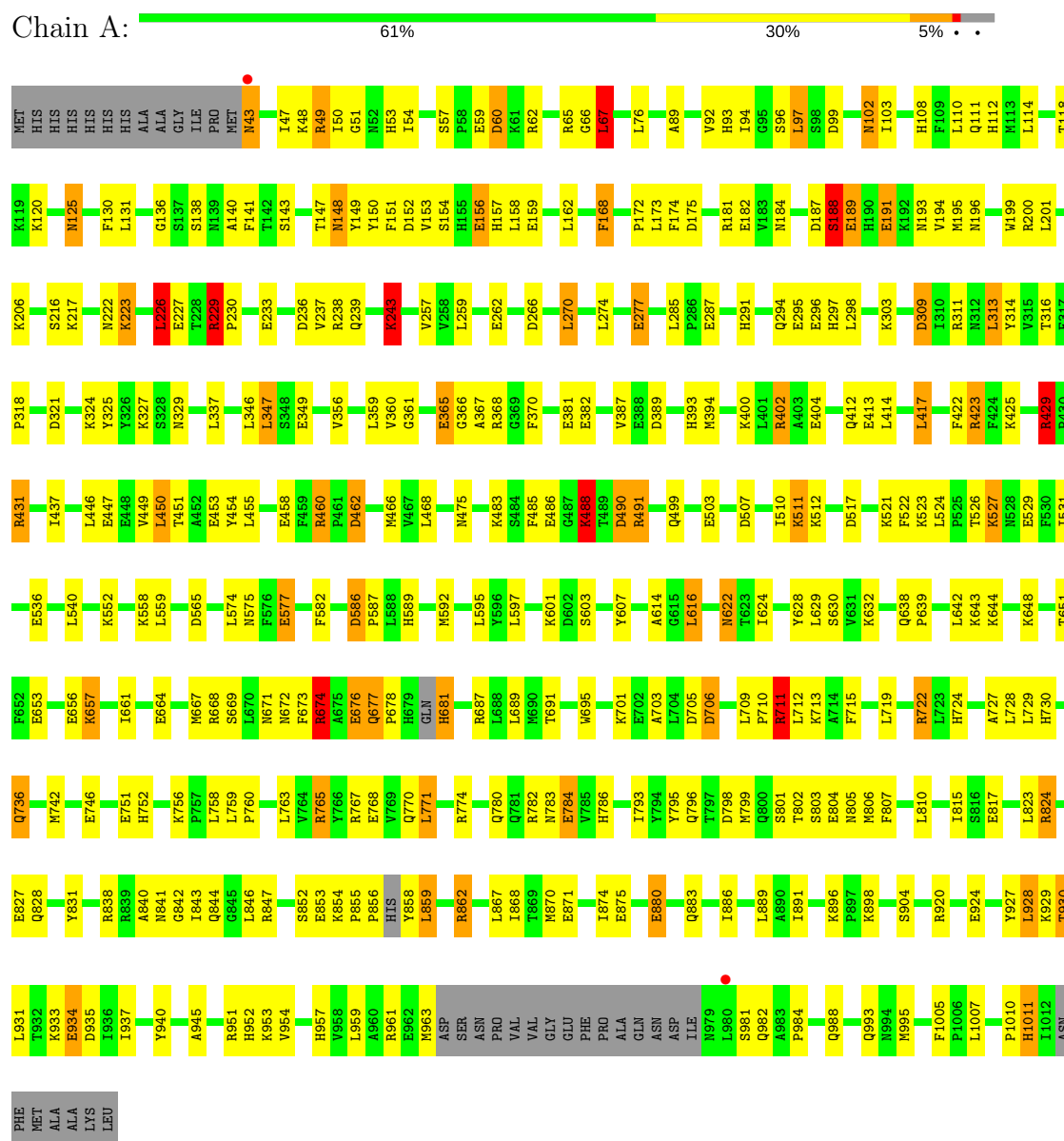
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	O	0	0
			1	1		
6	F	2	Total	O	0	0
			2	2		

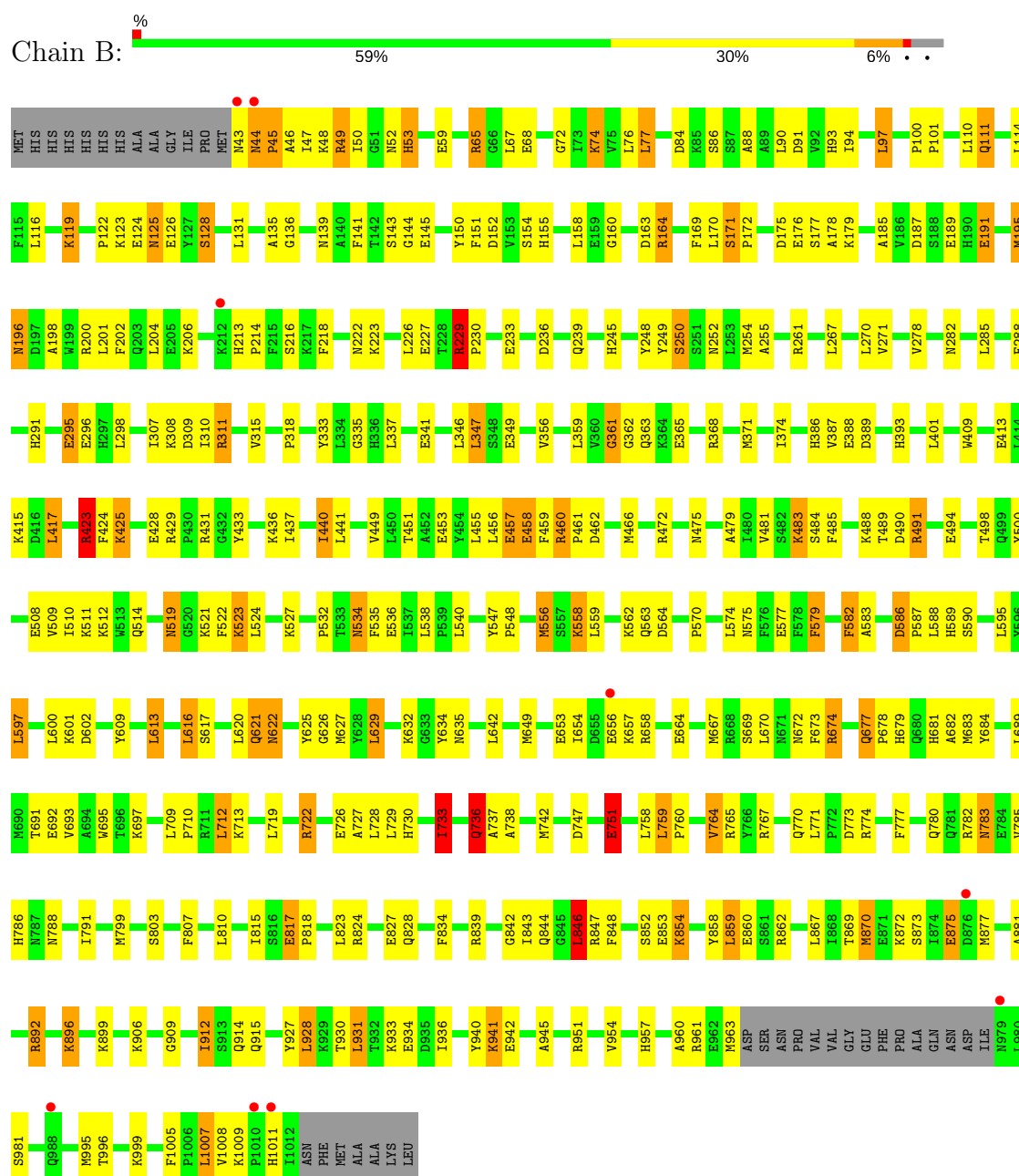
3 Residue-property plots

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

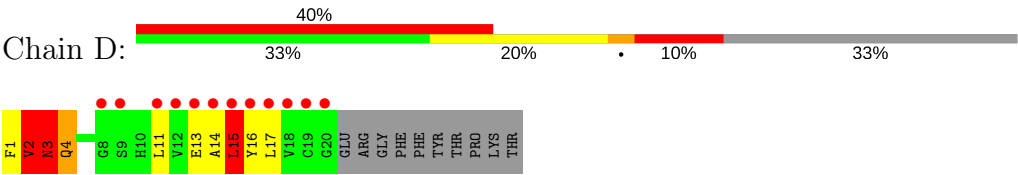
• Molecule 1: INSULIN-DEGRADING ENZYME



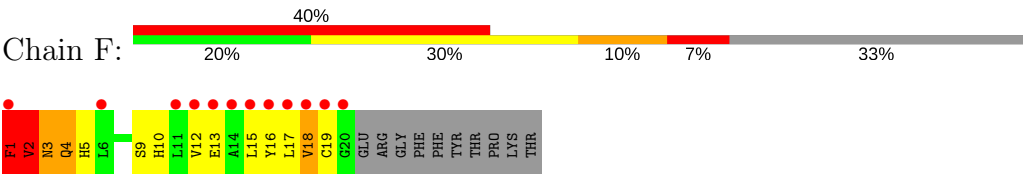
• Molecule 1: INSULIN-DEGRADING ENZYME



● Molecule 3: INSULIN B CHAIN



● Molecule 3: INSULIN B CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.17Å 263.17Å 90.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 2.80 29.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.85-2.80) 99.7 (29.85-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.220 0.181 , 0.225	Depositor DCC
R_{free} test set	4422 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16597	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, DIO

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	1.48	53/7973 (0.7%)	1.27	51/10784 (0.5%)
1	B	1.37	27/7985 (0.3%)	1.24	42/10805 (0.4%)
2	C	1.33	0/156	1.41	2/211 (0.9%)
2	E	1.10	1/156 (0.6%)	1.41	2/211 (0.9%)
3	D	1.66	0/156	1.68	5/211 (2.4%)
3	F	1.38	1/156 (0.6%)	2.00	8/211 (3.8%)
All	All	1.42	82/16582 (0.5%)	1.27	110/22433 (0.5%)

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
3	D	1	2
All	All	1	3

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ALA	CA-CB	-9.07	1.33	1.52
1	A	871	GLU	CG-CD	9.06	1.65	1.51
1	A	189	GLU	CD-OE1	8.43	1.34	1.25
1	B	189	GLU	CG-CD	8.25	1.64	1.51
1	A	458	GLU	CB-CG	-8.25	1.36	1.52

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	674	ARG	NE-CZ-NH1	16.35	128.47	120.30
3	F	1	PHE	N-CA-C	-14.93	70.69	111.00
1	A	586	ASP	CB-CG-OD1	13.06	130.05	118.30
1	B	460	ARG	NE-CZ-NH1	-11.26	114.67	120.30
3	F	2	VAL	N-CA-CB	-11.24	86.78	111.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	14	ALA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1010	PRO	Peptide
3	D	2	VAL	Peptide
3	D	3	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7781	0	7719	242	0
1	B	7790	0	7719	272	0
2	C	155	0	143	29	0
2	E	155	0	143	39	0
3	D	153	0	149	8	0
3	F	153	0	149	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	32	1	0
5	B	24	0	32	6	0
6	A	189	0	0	43	0
6	B	163	0	0	27	0
6	C	3	0	0	1	0
6	D	2	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16597	0	16086	551	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 17.

The worst 5 of 551 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:B:597:LEU:HA	6:B:2095:HOH:O	1.17	1.33
1:B:361:GLY:O	2:E:2:ILE:HA	1.29	1.24
6:A:2116:HOH:O	2:C:2:ILE:HG22	1.24	1.24
1:B:736:GLN:HB2	6:B:2123:HOH:O	1.07	1.23
1:A:243:LYS:HG3	6:A:2041:HOH:O	1.38	1.21

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	945/990 (96%)	882 (93%)	60 (6%)	3 (0%)	43	75
1	B	951/990 (96%)	896 (94%)	51 (5%)	4 (0%)	36	70
2	C	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
2	E	19/21 (90%)	15 (79%)	4 (21%)	0	100	100
3	D	18/30 (60%)	16 (89%)	2 (11%)	0	100	100
3	F	18/30 (60%)	17 (94%)	1 (6%)	0	100	100
All	All	1970/2082 (95%)	1843 (94%)	120 (6%)	7 (0%)	36	70

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	PRO
1	A	1011	HIS
1	B	295	GLU
1	B	751	GLU
1	A	488	LYS

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	846/879 (96%)	755 (89%)	91 (11%)	7	21
1	B	846/879 (96%)	752 (89%)	94 (11%)	7	20
2	C	19/20 (95%)	15 (79%)	4 (21%)	1	3
2	E	19/20 (95%)	13 (68%)	6 (32%)	0	1
3	D	17/26 (65%)	12 (71%)	5 (29%)	0	1
3	F	17/26 (65%)	13 (76%)	4 (24%)	1	2
All	All	1764/1850 (95%)	1560 (88%)	204 (12%)	6	18

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	65	ARG
1	B	282	ASN
2	C	19	TYR
1	B	76	LEU
1	B	158	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	883	GLN
1	B	111	GLN
1	B	957	HIS
1	A	957	HIS

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Mol	Chain	Res	Type
1	B	52	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
5	DIO	A	3013	-	6,6,6	0.54	0	6,6,6	1.28	1 (16%)
5	DIO	A	3014	-	6,6,6	0.65	0	6,6,6	0.48	0
5	DIO	A	3015	-	6,6,6	0.62	0	6,6,6	1.24	1 (16%)
5	DIO	A	3016	-	6,6,6	0.46	0	6,6,6	0.98	0
5	DIO	B	3013	-	6,6,6	0.65	0	6,6,6	0.93	1 (16%)
5	DIO	B	3014	-	6,6,6	0.84	0	6,6,6	1.54	2 (33%)
5	DIO	B	3015	-	6,6,6	0.63	0	6,6,6	1.67	1 (16%)
5	DIO	B	3016	-	6,6,6	0.60	0	6,6,6	1.23	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
5	DIO	A	3013	-	-	0/0/6/6	0/1/1/1
5	DIO	A	3014	-	-	0/0/6/6	0/1/1/1
5	DIO	A	3015	-	-	0/0/6/6	0/1/1/1
5	DIO	A	3016	-	-	0/0/6/6	0/1/1/1
5	DIO	B	3013	-	-	0/0/6/6	0/1/1/1
5	DIO	B	3014	-	-	0/0/6/6	0/1/1/1
5	DIO	B	3015	-	-	0/0/6/6	0/1/1/1
5	DIO	B	3016	-	-	0/0/6/6	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3013	DIO	C2'-O1'-C1'	2.05	116.77	109.89
5	A	3013	DIO	C2'-O1'-C1'	2.29	117.60	109.89
5	A	3015	DIO	C2'-O1'-C1'	2.35	117.79	109.89
5	B	3014	DIO	C2-O1-C1	2.43	118.05	109.89
5	B	3014	DIO	C2'-O1'-C1'	2.73	119.06	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3014	DIO	1	0
5	B	3013	DIO	3	0
5	B	3014	DIO	1	0
5	B	3015	DIO	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 [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, 95th 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 ²)	Q<0.9
1	A	953/990 (96%)	-0.51	2 (0%) 94 94	23, 35, 51, 70	0
1	B	955/990 (96%)	-0.43	9 (0%) 84 79	25, 41, 57, 76	0
2	C	21/21 (100%)	2.73	14 (66%) 0 0	34, 53, 56, 57	0
2	E	21/21 (100%)	3.03	12 (57%) 0 0	33, 46, 65, 67	0
3	D	20/30 (66%)	3.02	12 (60%) 0 0	33, 62, 73, 75	0
3	F	20/30 (66%)	2.71	12 (60%) 0 0	43, 54, 58, 59	0
All	All	1990/2082 (95%)	-0.33	61 (3%) 49 38	23, 38, 56, 76	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	21	ASN	7.1
2	E	16	LEU	6.3
3	F	20	GLY	6.1
2	E	20	CYS	6.1
3	D	19	CYS	6.0

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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
5	DIO	B	3015	6/6	0.90	0.28	68,73,74,74	0
4	ZN	B	3012	1/1	0.91	0.30	2,2,2,2	0
4	ZN	A	3012	1/1	0.94	0.29	2,2,2,2	0
5	DIO	A	3016	6/6	0.95	0.20	71,72,74,74	0
5	DIO	B	3014	6/6	0.95	0.16	64,66,67,67	0
5	DIO	A	3013	6/6	0.95	0.18	61,63,65,66	0
5	DIO	B	3016	6/6	0.95	0.27	81,83,84,85	0
5	DIO	A	3014	6/6	0.95	0.25	54,57,59,60	0
5	DIO	A	3015	6/6	0.97	0.35	69,70,70,71	0
5	DIO	B	3013	6/6	0.97	0.23	50,53,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.