



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:13 AM GMT

PDB ID : 2WBY  
Title : CRYSTAL STRUCTURE OF HUMAN INSULIN-DEGRADING ENZYME  
IN COMPLEX WITH INSULIN  
Authors : Manolopoulou, M.; Guo, Q.; Malito, E.; Schilling, A.B.; Tang, W.J.  
Deposited on : 2009-03-06  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

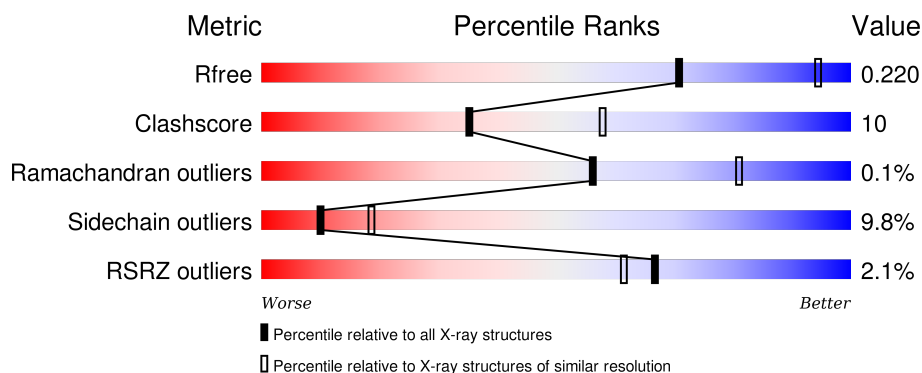
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	990	<div> <div>74%</div> <div>19%</div> <div>• • •</div> </div>
1	B	990	<div> <div>70%</div> <div>23%</div> <div>• •</div> </div>
2	C	20	<div> <div>30%</div> <div>80%</div> <div>20%</div> </div>
2	E	20	<div> <div>40%</div> <div>70%</div> <div>30%</div> </div>
3	D	19	<div> <div>42%</div> <div>63%</div> <div>21%</div> <div>11%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	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
4	ZN	A	3012	-	-	X	X
4	ZN	B	3012	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16926 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	958	Total	C	N	O	S	0	0	1
			7813	5032	1313	1445	23			
1	B	955	Total	C	N	O	S	0	0	1
			7787	5018	1307	1440	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	20	Total 155	C 95	N 23	O 33	S 4	0	0	0
2	E	20	Total 155	C 95	N 23	O 33	S 4	0	0	0

- Molecule 3 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total 143	C 94	N 24	O 24	S 1	0	0	0
3	F	19	Total 149	C 97	N 25	O 25	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	408	Total	O	0	0
			408	408		
5	B	295	Total	O	0	0
			295	295		
5	C	6	Total	O	0	0
			6	6		
5	D	4	Total	O	0	0
			4	4		
5	E	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	4	Total	O	0	0
			4	4		

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 ( $\text{RSRZ} > 2$ ). 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.

Chain A: 74% 19% 7%

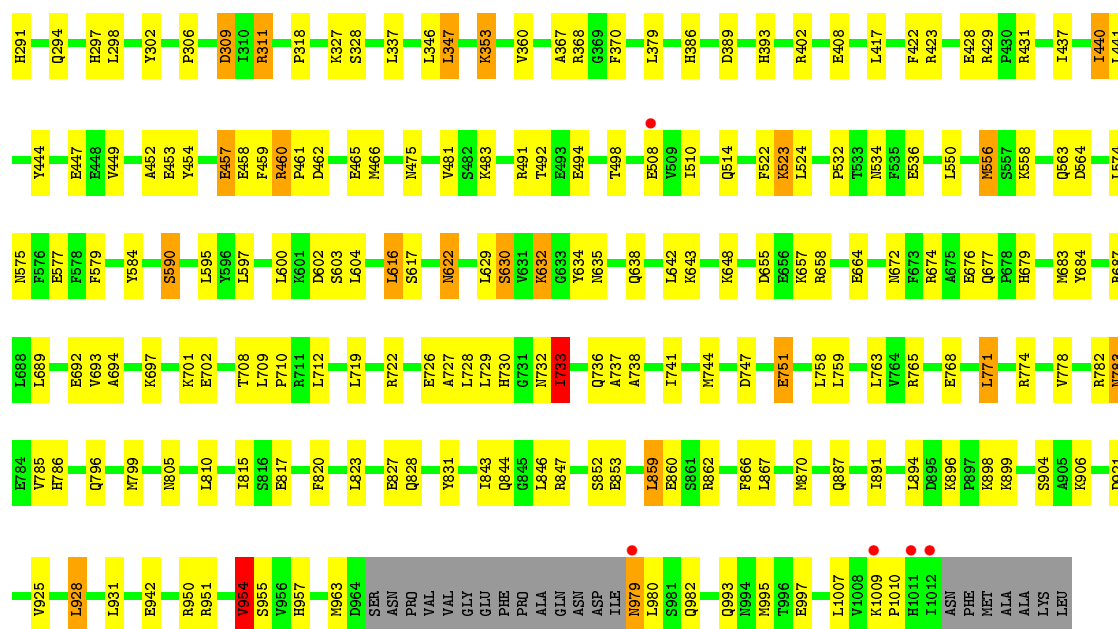
Chain	Conserved Amino Acids (%)
ASN	100%
PHE	100%
MET	100%
ALA	100%
LYS	100%
LEU	100%
ASN	100%
PHE	100%
MET	100%
ALA	100%
LYS	100%
LEU	100%
ASN	100%
PHE	100%
MET	100%
ALA	100%
LYS	100%
LEU	100%

Chain B:

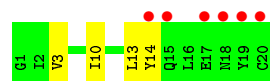
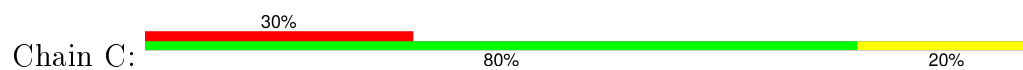
70% 23%

MET  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
ALA  
ALA  
GLY  
ILE  
PRO  
MET  
ASN  
N44  
P45  
R49  
I50  
G51  
N52  
H53  
K61  
R65  
G66  
L67  
I73  
K74  
V75  
L76  
L77  
H83  
L97  
N102  
H108  
F109  
L110  
Q111  
H112  
K119  
K123  
E124  
N125  
E126  
L131  
S132  
G136  
S137  
S138

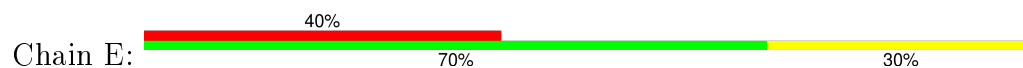
F141  
E145  
F151  
D152  
H156  
H157  
L158  
E159  
L162  
S171  
H184  
A195  
E189  
H190  
E191  
M196  
D197  
A198  
V199  
R200  
L201  
K223  
L226  
R229  
Q238  
Q239  
H245  
Y249  
S250  
S251  
L267  
L270  
V271  
V272  
K273  
N282  
L285  
P286  
E287  
F290



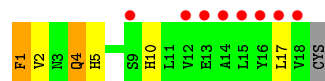
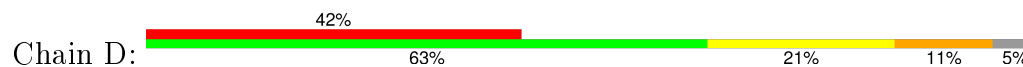
- Molecule 2: INSULIN A CHAIN



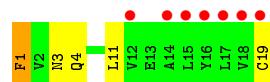
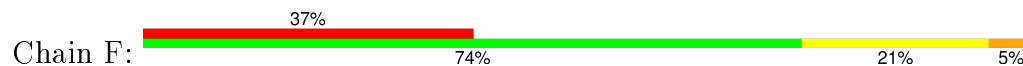
- Molecule 2: INSULIN A CHAIN



- 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, $\alpha$ , $\beta$ , $\gamma$	262.32Å 262.32Å 90.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.08 – 2.60 31.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.08-2.60) 99.9 (31.46-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.39 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.164 , 0.218 0.168 , 0.220	Depositor DCC
$R_{free}$ test set	5438 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.3	EDS
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 108878 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.21	22/8007 (0.3%)	1.09	34/10833 (0.3%)
1	B	1.19	21/7982 (0.3%)	1.04	31/10801 (0.3%)
2	C	1.25	0/156	1.11	0/209
2	E	1.22	0/156	1.04	0/209
3	D	1.55	3/146 (2.1%)	1.11	0/198
3	F	1.42	1/152 (0.7%)	1.03	0/206
All	All	1.20	47/16599 (0.3%)	1.06	65/22456 (0.3%)

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

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	GLU	CD-OE2	17.00	1.44	1.25
1	A	189	GLU	CD-OE1	15.73	1.43	1.25
1	A	189	GLU	CG-CD	8.99	1.65	1.51
1	A	577	GLU	CG-CD	8.46	1.64	1.51
1	B	508	GLU	CG-CD	8.38	1.64	1.51
1	B	74	LYS	CE-NZ	6.96	1.66	1.49
1	B	632	LYS	CD-CE	6.74	1.68	1.51
1	B	239	GLN	CG-CD	6.56	1.66	1.51
1	A	176	GLU	CG-CD	6.44	1.61	1.51
1	B	508	GLU	CB-CG	6.43	1.64	1.52
1	A	150	TYR	CD1-CE1	6.33	1.48	1.39
1	B	290	GLU	CG-CD	6.24	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	577	GLU	CG-CD	6.18	1.61	1.51
1	A	141	PHE	CD2-CE2	6.13	1.51	1.39
1	A	880	GLU	CG-CD	6.11	1.61	1.51
1	A	527	LYS	CG-CD	5.92	1.72	1.52
1	B	453	GLU	CB-CG	5.86	1.63	1.52
1	B	302	TYR	CD2-CE2	5.85	1.48	1.39
1	A	871	GLU	CG-CD	5.85	1.60	1.51
1	B	465	GLU	CG-CD	5.84	1.60	1.51
1	A	674	ARG	CG-CD	5.66	1.66	1.51
1	A	871	GLU	CD-OE1	5.63	1.31	1.25
1	A	159	GLU	CD-OE1	5.61	1.31	1.25
1	B	189	GLU	CG-CD	5.56	1.60	1.51
1	B	820	PHE	CE2-CZ	5.51	1.47	1.37
3	D	1	PHE	CB-CG	5.51	1.60	1.51
3	D	1	PHE	N-CA	5.49	1.57	1.46
1	A	237	VAL	CB-CG1	5.47	1.64	1.52
1	A	625	TYR	CE2-CZ	5.45	1.45	1.38
1	B	997	GLU	CG-CD	5.42	1.60	1.51
1	B	189	GLU	CD-OE1	5.34	1.31	1.25
1	B	630	SER	CB-OG	-5.32	1.35	1.42
3	D	1	PHE	CD2-CE2	5.30	1.49	1.39
1	A	582	PHE	CE2-CZ	5.29	1.47	1.37
1	B	408	GLU	CB-CG	5.29	1.62	1.52
1	B	453	GLU	CD-OE2	5.21	1.31	1.25
1	A	527	LYS	CB-CG	5.17	1.66	1.52
1	A	141	PHE	CD1-CE1	5.17	1.49	1.39
1	A	159	GLU	CD-OE2	5.16	1.31	1.25
1	B	422	PHE	CE2-CZ	5.16	1.47	1.37
1	A	447	GLU	CG-CD	5.14	1.59	1.51
3	F	1	PHE	N-CA	5.12	1.56	1.46
1	A	577	GLU	CB-CG	5.08	1.61	1.52
1	A	834	PHE	CE1-CZ	5.04	1.47	1.37
1	B	191	GLU	CD-OE1	5.03	1.31	1.25
1	A	395	PHE	CE1-CZ	5.03	1.47	1.37
1	B	428	GLU	CG-CD	5.00	1.59	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	GLU	CG-CD-OE2	-14.71	88.88	118.30
1	A	189	GLU	CG-CD-OE1	13.60	145.50	118.30
1	B	189	GLU	CG-CD-OE1	-11.84	94.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	B	189	GLU	CG-CD-OE2	9.24	136.78	118.30
1	B	229	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	838	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	A	311	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	B	52	ASN	N-CA-C	8.48	133.90	111.00
1	A	892	ARG	NE-CZ-NH2	8.45	124.53	120.30
1	A	65	ARG	NE-CZ-NH1	-8.29	116.15	120.30
1	B	52	ASN	CB-CA-C	-8.28	93.84	110.40
1	A	460	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	586	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	694	ALA	CB-CA-C	7.42	121.22	110.10
1	B	460	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	B	311	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	711	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	954	VAL	CB-CA-C	-6.99	98.11	111.40
1	B	360	VAL	CB-CA-C	-6.92	98.25	111.40
1	A	597	LEU	CB-CG-CD1	6.74	122.45	111.00
1	B	223	LYS	CD-CE-NZ	-6.57	96.58	111.70
1	B	954	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	152	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	402	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	655	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	636	ASP	N-CA-C	6.25	127.87	111.00
1	A	862	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	636	ASP	CB-CA-C	-6.22	97.96	110.40
1	B	460	ARG	CG-CD-NE	-6.12	98.96	111.80
1	A	862	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	226	LEU	CB-CG-CD1	6.07	121.31	111.00
1	A	892	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	767	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	311	ARG	CB-CA-C	5.79	121.97	110.40
1	B	431	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	928	LEU	CB-CA-C	-5.77	99.23	110.20
1	B	452	ALA	C-N-CA	-5.76	107.30	121.70
1	A	65	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	B	733	ILE	CB-CA-C	-5.58	100.44	111.60
1	B	238	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	181	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	462	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	763	LEU	CB-CG-CD1	5.48	120.31	111.00
1	B	229	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	823	LEU	CB-CG-CD1	5.43	120.23	111.00
1	A	67	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	637	LYS	N-CA-CB	5.39	120.30	110.60
1	A	553	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	490	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	565	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	431	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	239	GLN	CA-CB-CG	5.25	124.96	113.40
1	A	217	LYS	CD-CE-NZ	-5.23	99.67	111.70
1	A	510	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	B	311	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	928	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	674	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	309	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	687	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	951	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	604	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	538	LEU	CA-CB-CG	-5.08	103.61	115.30
1	B	453	GLU	CB-CA-C	5.04	120.48	110.40
1	B	564	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	979	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	7813	0	7744	146	0
1	B	7787	0	7715	161	0
2	C	155	0	144	4	0
2	E	155	0	143	7	0
3	D	143	0	142	13	0
3	F	149	0	146	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	2	0
4	B	1	0	0	3	0
5	A	408	0	0	24	0
5	B	295	0	0	14	0
5	C	6	0	0	0	0
5	D	4	0	0	1	0
5	E	5	0	0	0	0
5	F	4	0	0	0	0
All	All	16926	0	16034	316	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 10.

All (316) 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:491:ARG:HG3	1:A:491:ARG:HH11	1.02	1.17
4:B:3012:ZN:ZN	3:F:1:PHE:N	1.11	1.14
4:A:3012:ZN:ZN	3:D:1:PHE:N	1.17	1.06
1:B:189:GLU:OE2	3:F:1:PHE:N	1.90	1.03
1:B:119:LYS:HE3	1:B:171:SER:HB2	1.44	0.98
1:B:189:GLU:OE2	4:B:3012:ZN:ZN	1.11	0.97
1:A:491:ARG:CG	1:A:491:ARG:HH11	1.75	0.97
1:A:431:ARG:HD3	5:A:2206:HOH:O	1.64	0.96
1:A:189:GLU:OE1	3:D:1:PHE:N	1.98	0.96
1:A:764:VAL:HA	5:A:2305:HOH:O	1.67	0.92
1:A:674:ARG:HD3	5:A:2321:HOH:O	1.68	0.91
1:A:423:ARG:CG	1:A:423:ARG:HH11	1.84	0.90
1:A:102:ASN:HD22	1:A:102:ASN:H	1.20	0.89
2:E:4:GLU:HG3	3:F:11:LEU:HD22	1.55	0.89
1:A:491:ARG:NH1	1:A:491:ARG:HG3	1.80	0.89
4:A:3012:ZN:ZN	3:D:1:PHE:H2	0.80	0.86
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.27	0.83
1:B:125:ASN:H	1:B:125:ASN:HD22	1.26	0.83
1:B:77:LEU:HD21	1:B:271:VAL:HG11	1.61	0.82
1:A:316:THR:HG23	5:A:2131:HOH:O	1.80	0.81
1:B:622:ASN:H	1:B:622:ASN:HD22	1.28	0.81
1:A:711:ARG:HH21	1:A:711:ARG:HG2	1.46	0.80
1:B:440:ILE:HD11	1:B:449:VAL:HB	1.64	0.80
1:B:102:ASN:H	1:B:102:ASN:HD22	1.30	0.79
1:A:199:TRP:HA	3:D:4:GLN:HE22	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLN:H	1:B:297:HIS:HD2	1.29	0.78
1:A:294:GLN:H	1:A:297:HIS:HD2	1.27	0.78
1:A:423:ARG:HG3	1:A:423:ARG:HH11	1.48	0.78
1:A:196:ASN:HD22	1:A:199:TRP:H	1.29	0.78
1:B:783:ASN:HD22	1:B:785:VAL:H	1.32	0.77
1:B:108:HIS:NE2	1:B:189:GLU:OE2	2.18	0.77
1:B:771:LEU:HD21	1:B:954:VAL:HG22	1.65	0.77
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.65	0.77
1:A:771:LEU:HD21	1:A:954:VAL:HG22	1.65	0.76
2:E:10:ILE:HG23	3:F:3:ASN:HB3	1.67	0.76
1:A:125:ASN:HD22	1:A:125:ASN:H	1.32	0.76
1:B:368:ARG:HD2	5:B:2125:HOH:O	1.85	0.75
1:A:521:LYS:NZ	5:A:2231:HOH:O	2.17	0.75
1:B:494:GLU:HG2	5:B:2170:HOH:O	1.86	0.75
1:A:934:GLU:HG2	1:B:53:HIS:CE1	2.22	0.74
1:A:53:HIS:HE1	5:A:2012:HOH:O	1.71	0.74
1:A:429:ARG:HB2	2:C:14:TYR:OH	1.87	0.74
1:A:470:LYS:HE3	5:A:2215:HOH:O	1.86	0.74
1:B:49:ARG:NH2	1:B:447:GLU:OE1	2.21	0.73
1:A:309:ASP:H	1:A:672:ASN:HD21	1.35	0.73
1:B:309:ASP:H	1:B:672:ASN:HD21	1.36	0.73
1:B:51:GLY:N	1:B:66:GLY:O	2.20	0.73
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.87	0.73
1:A:636:ASP:OD2	1:A:636:ASP:O	2.07	0.73
1:A:316:THR:CG2	5:A:2131:HOH:O	2.34	0.72
1:A:927:TYR:O	1:A:930:THR:HB	1.90	0.72
1:B:579:PHE:HE2	1:B:765:ARG:NH1	1.87	0.72
1:A:389:ASP:O	1:A:393:HIS:HD2	1.72	0.72
1:B:386:HIS:HE1	5:B:2132:HOH:O	1.72	0.72
1:B:782:ARG:NH2	1:B:963:MET:O	2.23	0.71
1:A:309:ASP:H	1:A:672:ASN:ND2	1.89	0.70
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.72	0.70
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.73	0.70
1:A:730:HIS:HD2	1:A:904:SER:OG	1.75	0.70
1:B:309:ASP:H	1:B:672:ASN:ND2	1.91	0.69
1:A:879:GLU:HG3	5:A:2362:HOH:O	1.92	0.69
4:B:3012:ZN:ZN	3:F:1:PHE:H1	1.02	0.69
1:A:880:GLU:HG3	1:B:457:GLU:HG2	1.75	0.69
2:C:10:ILE:HG12	3:D:4:GLN:O	1.93	0.68
1:A:950:ARG:HD2	5:A:2312:HOH:O	1.94	0.68
1:B:676:GLU:HA	1:B:676:GLU:OE2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:ASN:HD22	1:A:785:VAL:H	1.42	0.66
1:A:329:ASN:HD21	1:A:363:GLN:HE22	1.43	0.66
1:B:579:PHE:CE2	1:B:765:ARG:NH1	2.63	0.66
1:B:267:LEU:O	1:B:271:VAL:HG12	1.95	0.66
1:A:783:ASN:ND2	1:A:785:VAL:H	1.93	0.66
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.42	0.65
1:B:112:HIS:NE2	3:F:1:PHE:N	2.44	0.65
1:A:491:ARG:CD	5:A:2219:HOH:O	2.45	0.65
1:A:229:ARG:HD2	1:A:233:GLU:OE2	1.97	0.65
1:A:622:ASN:H	1:A:622:ASN:HD22	1.44	0.64
1:A:189:GLU:OE2	3:D:1:PHE:HA	1.98	0.64
1:A:423:ARG:NH1	1:A:423:ARG:CG	2.56	0.64
1:B:783:ASN:ND2	1:B:785:VAL:H	1.96	0.64
1:A:491:ARG:HD2	5:A:2219:HOH:O	1.98	0.63
1:B:906:LYS:HE2	1:B:921:ASP:OD2	1.98	0.63
1:B:979:ASN:N	1:B:979:ASN:HD22	1.95	0.63
1:B:632:LYS:NZ	5:B:2213:HOH:O	2.11	0.63
1:A:782:ARG:NH1	1:A:963:MET:O	2.30	0.63
1:B:108:HIS:NE2	3:F:1:PHE:N	2.41	0.63
3:D:4:GLN:HG3	3:D:5:HIS:N	2.14	0.63
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.27	0.62
1:A:316:THR:HB	1:A:374:ILE:HG22	1.80	0.62
1:B:112:HIS:NE2	1:B:189:GLU:OE2	2.33	0.62
1:A:102:ASN:ND2	1:A:102:ASN:H	1.97	0.62
1:A:112:HIS:NE2	3:D:1:PHE:N	2.49	0.61
1:A:827:GLU:OE1	1:A:862:ARG:HD3	2.01	0.61
1:B:125:ASN:N	1:B:125:ASN:HD22	1.96	0.61
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.13	0.60
1:B:847:ARG:NH1	5:B:2257:HOH:O	2.09	0.60
1:B:306:PRO:O	1:B:483:LYS:HE3	2.01	0.60
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.00	0.60
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.84	0.60
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.84	0.60
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.31	0.60
1:B:491:ARG:HD2	5:B:2167:HOH:O	2.02	0.59
1:B:294:GLN:H	1:B:297:HIS:CD2	2.14	0.59
1:B:783:ASN:ND2	1:B:786:HIS:H	2.01	0.59
1:A:783:ASN:ND2	1:A:786:HIS:H	2.00	0.59
1:B:108:HIS:CE1	1:B:189:GLU:OE2	2.56	0.59
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.03	0.58
1:B:162:LEU:HD23	1:B:270:LEU:CD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:LEU:HB2	1:B:796:GLN:OE1	2.04	0.58
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.86	0.58
1:B:184:ASN:HD21	1:B:223:LYS:HZ3	1.50	0.58
1:A:964:ASP:O	1:A:965:SER:CB	2.51	0.57
1:A:432:GLY:HA3	2:C:14:TYR:CE1	2.40	0.57
2:E:4:GLU:HG3	3:F:11:LEU:CD2	2.33	0.57
1:A:49:ARG:NH1	5:A:2005:HOH:O	2.38	0.57
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.86	0.57
1:A:566:LYS:O	1:A:568:PHE:CD1	2.56	0.57
1:A:789:SER:HB2	1:A:958:VAL:O	2.03	0.56
1:A:622:ASN:H	1:A:622:ASN:ND2	2.03	0.56
1:B:298:LEU:HD13	1:B:475:ASN:CB	2.36	0.56
1:B:110:LEU:HD23	1:B:110:LEU:C	2.25	0.56
1:A:898:LYS:HE3	5:A:2026:HOH:O	2.04	0.55
1:B:49:ARG:HG2	1:B:50:ILE:N	2.21	0.55
1:B:196:ASN:HD22	1:B:199:TRP:H	1.52	0.55
1:A:67:LEU:N	1:A:67:LEU:HD23	2.21	0.55
1:A:934:GLU:OE1	1:B:53:HIS:HE1	1.90	0.55
1:A:125:ASN:HD22	1:A:125:ASN:N	2.03	0.55
1:B:67:LEU:HB2	1:B:75:VAL:HB	1.89	0.55
1:B:622:ASN:H	1:B:622:ASN:ND2	2.01	0.54
1:A:431:ARG:CD	5:A:2206:HOH:O	2.36	0.54
1:B:602:ASP:OD1	1:B:658:ARG:CD	2.55	0.54
1:A:815:ILE:CG2	1:A:870:MET:HG3	2.36	0.54
1:A:711:ARG:HH21	1:A:711:ARG:CG	2.18	0.54
1:A:112:HIS:CE1	1:A:189:GLU:OE1	2.57	0.53
1:A:229:ARG:HG2	5:A:2101:HOH:O	2.08	0.53
1:B:386:HIS:CE1	5:B:2132:HOH:O	2.53	0.53
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.44	0.53
1:A:423:ARG:HG2	1:A:423:ARG:HH11	1.69	0.53
1:B:815:ILE:HG22	1:B:870:MET:HG3	1.90	0.53
1:B:575:ASN:OD1	1:B:630:SER:HB3	2.08	0.53
1:A:799:MET:CE	1:A:1008:VAL:HG22	2.39	0.53
1:B:906:LYS:CE	1:B:921:ASP:OD2	2.57	0.53
2:E:10:ILE:CG2	3:F:3:ASN:HB3	2.37	0.53
1:B:708:THR:HB	1:B:710:PRO:HD2	1.90	0.53
1:A:393:HIS:HE1	5:A:2155:HOH:O	1.91	0.52
1:B:196:ASN:ND2	1:B:198:ALA:H	2.06	0.52
1:B:185:ALA:HB2	1:B:828:GLN:HE22	1.74	0.52
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.91	0.52
1:A:491:ARG:CG	1:A:491:ARG:NH1	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:LYS:HB3	1:B:726:GLU:HG3	1.91	0.52
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.40	0.52
1:A:771:LEU:HB2	1:A:796:GLN:OE1	2.10	0.52
1:B:679:HIS:O	1:B:683:MET:HG3	2.09	0.52
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.10	0.52
1:A:316:THR:HG22	5:A:2169:HOH:O	2.10	0.52
1:A:222:ASN:O	1:A:226:LEU:HB2	2.10	0.52
1:B:76:LEU:HD12	1:B:437:ILE:HG21	1.91	0.52
1:B:49:ARG:CG	1:B:50:ILE:N	2.71	0.51
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.58	0.51
1:B:768:GLU:HB3	1:B:843:ILE:HG13	1.92	0.51
1:B:52:ASN:C	1:B:53:HIS:ND1	2.64	0.51
1:B:189:GLU:HG3	1:B:831:TYR:CE1	2.46	0.51
1:B:563:GLN:HG3	1:B:733:ILE:O	2.10	0.51
1:B:440:ILE:HD11	1:B:449:VAL:CB	2.39	0.51
1:B:979:ASN:ND2	1:B:979:ASN:N	2.58	0.51
1:B:162:LEU:HD23	1:B:270:LEU:HD11	1.91	0.51
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.10	0.51
1:A:90:LEU:HD12	1:A:256:VAL:HG22	1.93	0.51
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.39	0.51
1:B:429:ARG:HH11	1:B:429:ARG:HG2	1.74	0.51
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.58	0.51
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.93	0.50
2:E:3:VAL:HG23	2:E:3:VAL:O	2.11	0.50
1:A:102:ASN:HD22	1:A:102:ASN:N	1.95	0.50
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.40	0.50
1:B:440:ILE:HG12	1:B:444:TYR:HD2	1.76	0.50
1:A:294:GLN:H	1:A:297:HIS:CD2	2.19	0.50
1:B:196:ASN:ND2	1:B:199:TRP:H	2.09	0.50
1:A:196:ASN:ND2	1:A:199:TRP:H	2.06	0.50
1:A:771:LEU:HB3	1:A:952:HIS:HB3	1.93	0.50
1:B:402:ARG:NH2	5:B:2140:HOH:O	2.42	0.50
1:A:596:TYR:CD2	1:A:597:LEU:HD13	2.47	0.49
1:B:664:GLU:HB3	5:B:2219:HOH:O	2.10	0.49
1:B:510:ILE:O	1:B:514:GLN:HG3	2.12	0.49
1:B:534:ASN:ND2	1:B:536:GLU:H	2.10	0.49
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.61	0.49
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.47	0.49
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.43	0.49
1:A:961:ARG:HD2	1:A:962:GLU:OE1	2.12	0.49
1:A:812:ALA:O	1:A:816:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HD23	1:A:359:LEU:C	2.33	0.48
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.43	0.48
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.13	0.48
1:B:860:GLU:OE2	1:B:957:HIS:CE1	2.67	0.48
1:A:389:ASP:O	1:A:393:HIS:CD2	2.61	0.48
1:B:575:ASN:O	1:B:727:ALA:HA	2.14	0.48
1:B:603:SER:OG	1:B:648:LYS:HE3	2.13	0.48
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.94	0.48
1:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.57	0.48
1:B:729:LEU:HD12	1:B:738:ALA:HB1	1.95	0.48
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.95	0.48
1:A:799:MET:HE3	1:A:1008:VAL:CG2	2.44	0.48
1:B:189:GLU:OE1	3:F:1:PHE:HA	2.13	0.47
1:A:575:ASN:ND2	1:A:630:SER:OG	2.48	0.47
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.48	0.47
1:B:622:ASN:N	1:B:622:ASN:HD22	2.07	0.47
1:B:866:PHE:CZ	1:B:870:MET:HG2	2.50	0.47
1:B:747:ASP:O	1:B:751:GLU:HB2	2.15	0.47
1:B:311:ARG:HG3	1:B:379:LEU:HB2	1.96	0.47
1:B:93:HIS:HD2	1:B:145:GLU:O	1.98	0.46
1:A:566:LYS:O	1:A:568:PHE:CE1	2.68	0.46
1:B:556:MET:HA	1:B:556:MET:CE	2.46	0.46
1:B:774:ARG:HG2	1:B:774:ARG:HH11	1.81	0.46
1:A:450:LEU:HB2	5:A:2209:HOH:O	2.15	0.46
1:B:550:LEU:HD11	1:B:558:LYS:HG2	1.96	0.46
2:C:3:VAL:O	2:C:3:VAL:HG23	2.15	0.46
1:A:140:ALA:HA	1:A:148:ASN:O	2.16	0.46
1:A:319:ILE:HB	1:A:320:PRO:HD2	1.97	0.46
1:A:730:HIS:CD2	1:A:904:SER:OG	2.62	0.46
1:A:783:ASN:HD22	1:A:786:HIS:H	1.62	0.46
1:A:67:LEU:CD2	1:A:67:LEU:N	2.79	0.46
1:A:799:MET:HE1	1:A:1008:VAL:HA	1.98	0.46
1:A:586:ASP:OD1	1:A:589:HIS:HD2	1.99	0.46
1:B:778:VAL:HG22	1:B:955:SER:HB2	1.98	0.46
1:B:328:SER:HB2	1:B:458:GLU:O	2.16	0.46
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.97	0.45
1:B:245:HIS:O	1:B:249:TYR:HB2	2.16	0.45
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.98	0.45
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.47	0.45
1:A:48:LYS:O	1:A:49:ARG:HB3	2.17	0.45
1:B:347:LEU:HA	1:B:347:LEU:HD23	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:GLU:OE2	1:A:957:HIS:HE1	2.00	0.45
3:D:4:GLN:HE21	3:D:4:GLN:HB2	1.53	0.45
3:D:4:GLN:HG3	3:D:5:HIS:H	1.81	0.45
1:A:938:LYS:HE2	1:A:938:LYS:HB3	1.24	0.45
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.52	0.45
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.98	0.45
1:A:345:SER:OG	1:A:348:SER:HB3	2.17	0.45
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.99	0.44
1:B:52:ASN:O	1:B:53:HIS:ND1	2.50	0.44
1:B:102:ASN:H	1:B:102:ASN:ND2	2.07	0.44
1:B:635:ASN:OD1	1:B:732:ASN:ND2	2.47	0.44
1:A:507:ASP:O	1:A:511:LYS:HD3	2.18	0.44
1:A:172:PRO:HG2	1:A:174:PHE:CE1	2.52	0.44
1:B:389:ASP:O	1:B:393:HIS:HD2	2.00	0.44
1:B:730:HIS:HD2	1:B:904:SER:OG	2.00	0.44
1:B:196:ASN:ND2	1:B:198:ALA:N	2.65	0.44
1:A:880:GLU:OE1	1:B:327:LYS:HE3	2.18	0.43
1:B:162:LEU:HD23	1:B:270:LEU:HD13	1.99	0.43
1:B:44:ASN:HB3	1:B:45:PRO:HB3	2.00	0.43
1:B:894:LEU:HG	1:B:925:VAL:HG21	2.00	0.43
1:A:196:ASN:HD21	1:A:198:ALA:HB3	1.82	0.43
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.80	0.43
1:B:429:ARG:HD3	2:E:14:TYR:OH	2.18	0.43
1:A:806:MET:CE	1:A:928:LEU:HG	2.49	0.43
1:B:774:ARG:HG2	1:B:774:ARG:NH1	2.34	0.43
1:A:199:TRP:CH2	3:D:2:VAL:HG23	2.54	0.43
1:B:291:HIS:CE1	1:B:318:PRO:HB3	2.54	0.43
1:B:136:GLY:HA3	1:B:152:ASP:O	2.18	0.43
1:B:896:LYS:HB2	1:B:896:LYS:HE2	1.83	0.43
1:B:584:TYR:CD2	1:B:590:SER:HB2	2.54	0.43
1:A:526:THR:O	1:A:527:LYS:C	2.56	0.43
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.53	0.43
1:A:329:ASN:ND2	5:A:2142:HOH:O	2.52	0.43
1:B:151:PHE:C	1:B:151:PHE:CD1	2.92	0.43
1:A:43:ASN:ND2	5:A:2001:HOH:O	2.52	0.42
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.81	0.42
1:A:934:GLU:HG3	1:B:52:ASN:HB3	2.01	0.42
1:A:552:LYS:HE2	1:A:557:SER:OG	2.19	0.42
1:A:346:LEU:HD21	1:A:394:MET:HG2	2.01	0.42
1:A:491:ARG:NE	5:A:2219:HOH:O	2.51	0.42
1:B:622:ASN:N	1:B:622:ASN:ND2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:HE3	1:A:48:LYS:HB2	1.83	0.42
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.19	0.42
1:B:189:GLU:CD	3:F:1:PHE:HA	2.40	0.42
1:B:737:ALA:O	1:B:741:ILE:HG12	2.20	0.42
1:B:353:LYS:NZ	5:B:2120:HOH:O	2.52	0.42
1:B:125:ASN:N	1:B:125:ASN:ND2	2.67	0.42
1:A:198:ALA:HB1	3:D:4:GLN:OE1	2.20	0.42
1:B:574:LEU:O	1:B:630:SER:HA	2.20	0.42
1:B:950:ARG:HD2	1:B:950:ARG:HH11	1.72	0.42
1:A:457:GLU:HG2	5:A:2083:HOH:O	2.19	0.42
1:B:311:ARG:HA	1:B:481:VAL:O	2.19	0.42
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.55	0.42
1:A:304:ILE:HB	1:A:481:VAL:HG22	2.01	0.42
1:B:298:LEU:HD13	1:B:475:ASN:HB3	2.02	0.42
1:A:204:LEU:CD2	1:A:304:ILE:HD12	2.50	0.42
1:B:843:ILE:HG22	1:B:844:GLN:H	1.85	0.42
1:B:141:PHE:CD1	2:E:12:SER:HB3	2.55	0.42
1:A:423:ARG:HG2	1:A:423:ARG:NH1	2.29	0.41
1:A:711:ARG:HG2	1:A:711:ARG:NH2	2.22	0.41
1:A:756:LYS:HB3	1:A:757:PRO:HD2	2.02	0.41
3:D:10:HIS:CD2	5:D:2002:HOH:O	2.72	0.41
1:B:982:GLN:HA	5:B:2290:HOH:O	2.20	0.41
1:B:145:GLU:CD	1:B:367:ALA:HB1	2.40	0.41
1:A:446:LEU:O	1:A:449:VAL:HG22	2.20	0.41
1:A:683:MET:HA	1:A:792:GLU:OE2	2.19	0.41
1:A:114:LEU:HD13	1:A:168:PHE:HB3	2.01	0.41
1:B:522:PHE:C	1:B:523:LYS:HD3	2.41	0.41
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.55	0.41
1:A:123:LYS:HB3	1:A:126:GLU:HB2	2.03	0.41
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.85	0.41
1:A:594:TYR:HD1	1:A:622:ASN:HD21	1.68	0.41
1:B:768:GLU:OE1	5:B:2231:HOH:O	2.22	0.41
1:A:773:ASP:O	1:A:774:ARG:HB2	2.20	0.41
1:A:961:ARG:NH2	5:A:2396:HOH:O	2.52	0.41
1:B:159:GLU:OE2	1:B:273:LYS:NZ	2.51	0.41
1:B:200:ARG:NH2	1:B:498:THR:HA	2.34	0.41
1:B:65:ARG:HD3	5:B:2011:HOH:O	2.21	0.41
1:A:368:ARG:HD3	1:A:368:ARG:HH11	1.74	0.41
1:A:150:TYR:HD1	1:A:431:ARG:HG2	1.86	0.40
1:B:828:GLN:NE2	5:B:2246:HOH:O	2.54	0.40
1:B:689:LEU:HD23	1:B:995:MET:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:HIS:ND1	1:B:53:HIS:N	2.69	0.40
1:B:429:ARG:CG	1:B:429:ARG:NH1	2.83	0.40
1:B:429:ARG:NH1	1:B:429:ARG:HG2	2.36	0.40
1:A:118:THR:HG22	1:A:172:PRO:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	954/990 (96%)	918 (96%)	36 (4%)	0	100	100
1	B	951/990 (96%)	921 (97%)	29 (3%)	1 (0%)	56	81
2	C	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	E	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
3	D	16/19 (84%)	12 (75%)	4 (25%)	0	100	100
3	F	17/19 (90%)	17 (100%)	0	0	100	100
All	All	1974/2058 (96%)	1901 (96%)	72 (4%)	1 (0%)	56	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1010	PRO

### 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	848/879 (96%)	765 (90%)	83 (10%)	10	19
1	B	845/879 (96%)	761 (90%)	84 (10%)	10	18
2	C	19/19 (100%)	18 (95%)	1 (5%)	28	53
2	E	19/19 (100%)	18 (95%)	1 (5%)	28	53
3	D	16/17 (94%)	14 (88%)	2 (12%)	6	10
3	F	17/17 (100%)	15 (88%)	2 (12%)	6	12
All	All	1764/1830 (96%)	1591 (90%)	173 (10%)	10	19

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	61	LYS
1	A	67	LEU
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	120	LYS
1	A	125	ASN
1	A	148	ASN
1	A	158	LEU
1	A	192	LYS
1	A	201	LEU
1	A	226	LEU
1	A	229	ARG
1	A	270	LEU
1	A	285	LEU
1	A	290	GLU
1	A	316	THR
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	348	SER
1	A	356	VAL
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG

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Mol	Chain	Res	Type
1	A	446	LEU
1	A	449	VAL
1	A	450	LEU
1	A	466	MET
1	A	486	GLU
1	A	491	ARG
1	A	499	GLN
1	A	512	LYS
1	A	517	ASP
1	A	527	LYS
1	A	595	LEU
1	A	597	LEU
1	A	603	SER
1	A	612	GLU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	632	LYS
1	A	642	LEU
1	A	648	LYS
1	A	657	LYS
1	A	660	GLU
1	A	674	ARG
1	A	711	ARG
1	A	712	LEU
1	A	718	GLN
1	A	728	LEU
1	A	759	LEU
1	A	765	ARG
1	A	771	LEU
1	A	780	GLN
1	A	783	ASN
1	A	810	LEU
1	A	817	GLU
1	A	823	LEU
1	A	846	LEU
1	A	853	GLU
1	A	854	LYS
1	A	859	LEU
1	A	861	SER
1	A	867	LEU
1	A	871	GLU

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Mol	Chain	Res	Type
1	A	872	LYS
1	A	875	GLU
1	A	879	GLU
1	A	889	LEU
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	934	GLU
1	A	938	LYS
1	A	954	VAL
1	A	979	ASN
1	A	1007	LEU
1	A	1011	HIS
1	B	53	HIS
1	B	61	LYS
1	B	65	ARG
1	B	67	LEU
1	B	76	LEU
1	B	77	LEU
1	B	97	LEU
1	B	102	ASN
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	132	SER
1	B	156	GLU
1	B	158	LEU
1	B	196	ASN
1	B	201	LEU
1	B	223	LYS
1	B	226	LEU
1	B	229	ARG
1	B	270	LEU
1	B	271	VAL
1	B	282	ASN
1	B	285	LEU
1	B	287	GLU
1	B	337	LEU
1	B	347	LEU
1	B	353	LYS
1	B	417	LEU
1	B	423	ARG

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Mol	Chain	Res	Type
1	B	440	ILE
1	B	454	TYR
1	B	457	GLU
1	B	460	ARG
1	B	466	MET
1	B	492	THR
1	B	523	LYS
1	B	524	LEU
1	B	556	MET
1	B	590	SER
1	B	595	LEU
1	B	597	LEU
1	B	600	LEU
1	B	616	LEU
1	B	617	SER
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	643	LYS
1	B	657	LYS
1	B	677	GLN
1	B	701	LYS
1	B	702	GLU
1	B	712	LEU
1	B	719	LEU
1	B	722	ARG
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	744	MET
1	B	751	GLU
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	783	ASN
1	B	799	MET
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	846	LEU
1	B	853	GLU
1	B	859	LEU

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Mol	Chain	Res	Type
1	B	867	LEU
1	B	898	LYS
1	B	899	LYS
1	B	928	LEU
1	B	931	LEU
1	B	942	GLU
1	B	951	ARG
1	B	954	VAL
1	B	979	ASN
1	B	980	LEU
1	B	993	GLN
1	B	1007	LEU
1	B	1009	LYS
2	C	13	LEU
3	D	4	GLN
3	D	17	LEU
2	E	13	LEU
3	F	4	GLN
3	F	19	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	111	GLN
1	A	125	ASN
1	A	129	GLN
1	A	148	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	393	HIS
1	A	475	ASN
1	A	502	GLN

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Mol	Chain	Res	Type
1	A	515	ASN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	730	HIS
1	A	780	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	957	HIS
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	239	GLN
1	B	297	HIS
1	B	363	GLN
1	B	386	HIS
1	B	393	HIS
1	B	407	GLN
1	B	502	GLN
1	B	534	ASN
1	B	589	HIS
1	B	605	ASN
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	736	GLN
1	B	780	GLN
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	883	GLN
1	B	887	GLN
1	B	957	HIS
3	D	4	GLN

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Mol	Chain	Res	Type
3	F	4	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 2 ligands modelled in this entry, 2 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

### 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	958/990 (96%)	-0.70	5 (0%) 91 90	13, 24, 40, 71	0
1	B	955/990 (96%)	-0.63	7 (0%) 89 87	15, 28, 44, 78	0
2	C	20/20 (100%)	1.22	6 (30%) 1 0	22, 52, 60, 61	0
2	E	20/20 (100%)	1.41	8 (40%) 0 0	21, 46, 63, 67	0
3	D	18/19 (94%)	1.64	8 (44%) 0 0	26, 52, 56, 57	0
3	F	19/19 (100%)	1.60	7 (36%) 0 0	32, 49, 63, 64	0
All	All	1990/2058 (96%)	-0.58	41 (2%) 67 61	13, 26, 47, 78	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	16	TYR	6.7
3	F	16	TYR	5.6
2	E	20	CYS	5.5
2	E	19	TYR	4.7
3	F	19	CYS	4.4
2	C	19	TYR	4.4
3	D	15	LEU	4.1
3	F	17	LEU	3.9
2	C	18	ASN	3.8
2	E	17	GLU	3.7
2	C	20	CYS	3.7
3	D	14	ALA	3.6
3	F	18	VAL	3.5
3	F	15	LEU	3.4
2	E	14	TYR	3.3
1	B	52	ASN	3.2
1	B	45	PRO	3.1
2	E	16	LEU	3.1
2	E	18	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	15	GLN	2.8
3	F	14	ALA	2.8
1	B	979	ASN	2.7
1	A	43	ASN	2.6
2	C	17	GLU	2.5
3	D	12	VAL	2.5
3	D	9	SER	2.5
1	B	1012	ILE	2.4
3	D	13	GLU	2.4
1	A	42	MET	2.4
2	E	13	LEU	2.3
2	C	15	GLN	2.3
1	A	517	ASP	2.3
3	F	12	VAL	2.3
1	B	1011	HIS	2.2
2	C	14	TYR	2.2
1	A	964	ASP	2.2
3	D	17	LEU	2.1
3	D	18	VAL	2.1
1	A	1012	ILE	2.0
1	B	508	GLU	2.0
1	B	1009	LYS	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
4	ZN	A	3012	1/1	0.99	0.23	2.11	2,2,2,2	0
4	ZN	B	3012	1/1	0.98	0.21	0.78	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.