



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:18 AM GMT

PDB ID : 2WK3  
Title : CRYSTAL STRUCTURE OF HUMAN INSULIN-DEGRADING ENZYME  
IN COMPLEX WITH AMYLOID-BETA (1-42)  
Authors : Guo, Q.; Tang, W.J.  
Deposited on : 2009-06-05  
Resolution : 2.59 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

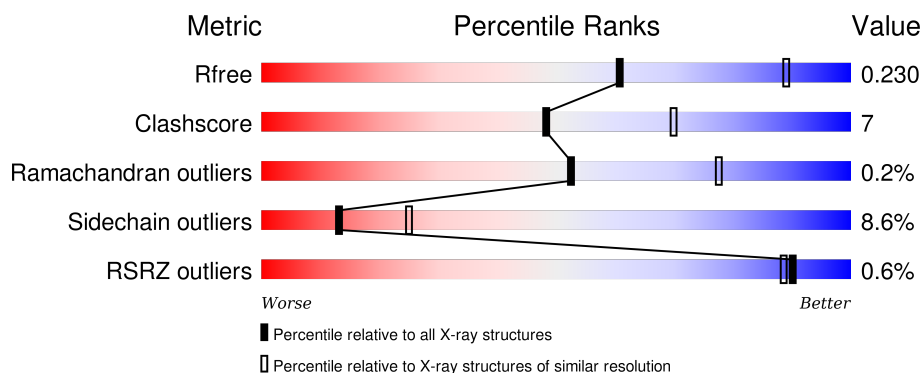
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	1019	
1	B	1019	
2	C	42	
2	D	42	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15911 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	7	1	0
			7773	5006	1304	1441	22			
1	B	956	Total	C	N	O	S	9	1	0
			7742	4992	1293	1435	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 BETA-AMYLOID PROTEIN 42.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			78	53	11	14			
2	D	10	Total	C	N	O	0	0	0
			82	55	11	16			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

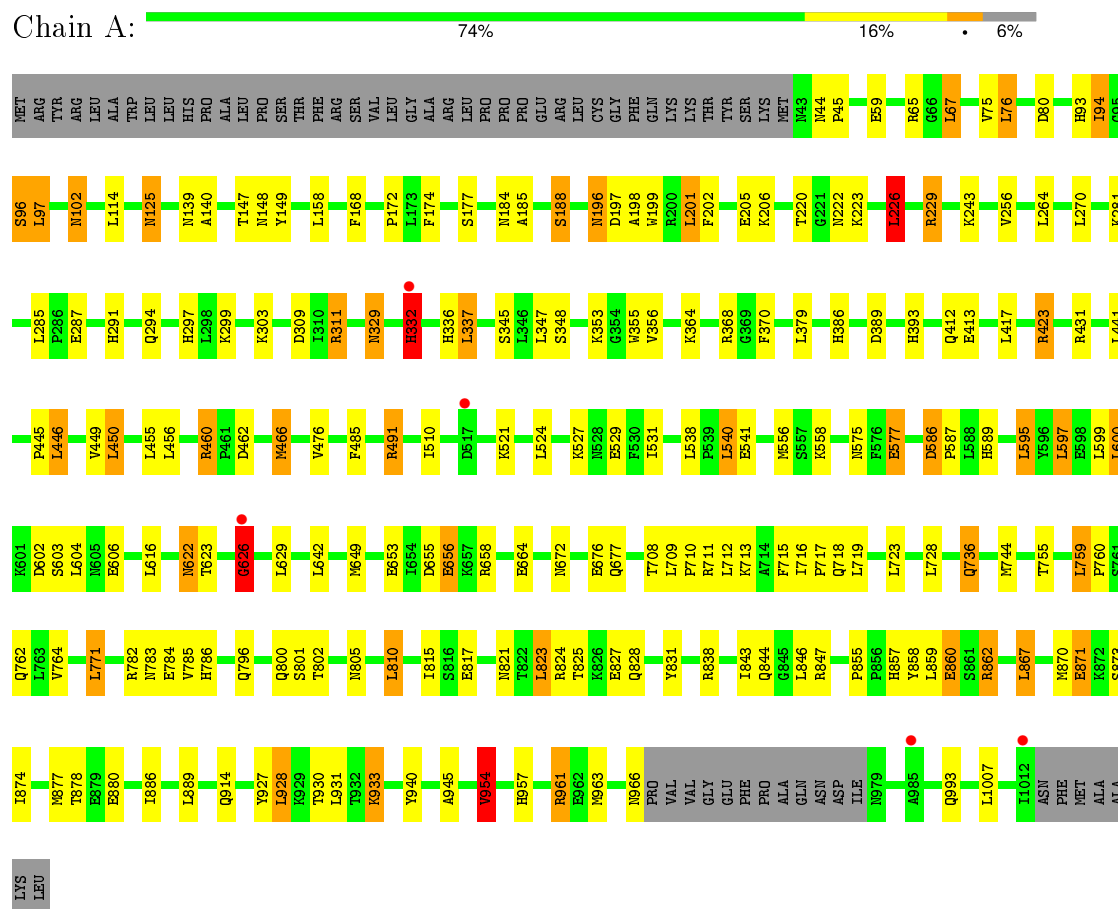
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	110	Total	O	0	0
			110	110		

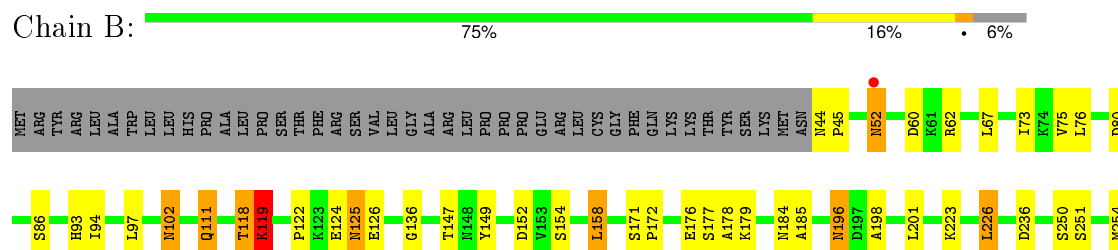
### 3 Residue-property plots

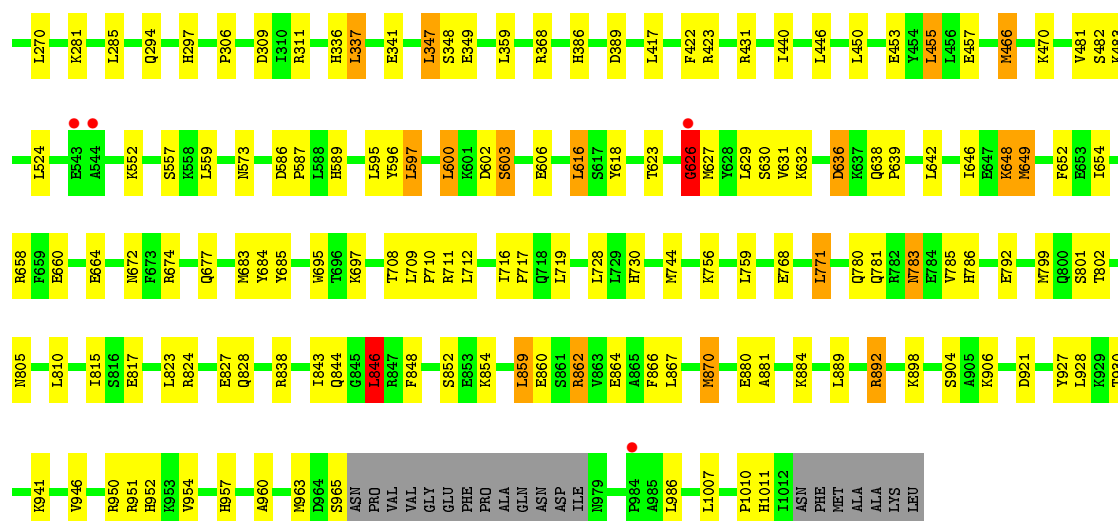
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: INSULIN DEGRADING ENZYME



#### • Molecule 1: INSULIN DEGRADING ENZYME





• Molecule 2: BETA-AMYLOID PROTEIN 42



• Molecule 2: BETA-AMYLOID PROTEIN 42



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	261.63 Å   261.63 Å   90.67 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	49.44 – 2.59 49.44 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.44-2.59) 99.9 (49.44-2.59)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.187 , 0.232 0.186 , 0.230	Depositor DCC
$R_{free}$ test set	5511 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.7	EDS
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 110150 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15911	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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	1.12	11/7972 (0.1%)	1.01	26/10801 (0.2%)
1	B	1.06	7/7937 (0.1%)	1.00	15/10754 (0.1%)
2	C	1.64	0/78	1.30	1/102 (1.0%)
2	D	1.72	0/82	1.28	1/107 (0.9%)
All	All	1.10	18/16069 (0.1%)	1.01	43/21764 (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
1	B	0	3
All	All	0	4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	453	GLU	CB-CG	7.44	1.66	1.52
1	A	332[A]	HIS	CA-C	6.88	1.70	1.52
1	A	332[B]	HIS	CA-C	6.88	1.70	1.52
1	A	676	GLU	CG-CD	6.53	1.61	1.51
1	A	577	GLU	CD-OE2	6.41	1.32	1.25
1	A	880	GLU	CG-CD	6.31	1.61	1.51
1	B	965	SER	CA-CB	6.20	1.62	1.52
1	A	871	GLU	CG-CD	6.14	1.61	1.51
1	B	422	PHE	CE2-CZ	5.97	1.48	1.37
1	A	287	GLU	CG-CD	5.58	1.60	1.51
1	A	527	LYS	CA-CB	5.48	1.66	1.53
1	B	126	GLU	CB-CG	5.45	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	ARG	CG-CD	5.39	1.65	1.51
1	A	606	GLU	CB-CG	-5.35	1.42	1.52
1	B	453	GLU	CG-CD	5.20	1.59	1.51
1	B	660	GLU	CG-CD	5.18	1.59	1.51
1	A	96	SER	CB-OG	-5.15	1.35	1.42
1	A	954	VAL	CB-CG2	-5.08	1.42	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	LYS	N-CA-CB	-24.65	66.22	110.60
1	B	52	ASN	N-CA-C	13.51	147.49	111.00
1	B	119	LYS	CB-CA-C	-10.65	89.10	110.40
1	A	847	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	311	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	B	52	ASN	CB-CA-C	-8.16	94.08	110.40
1	A	626	GLY	C-N-CA	8.11	141.99	121.70
1	A	626	GLY	N-CA-C	-8.09	92.87	113.10
2	D	17	LEU	CA-CB-CG	7.95	133.59	115.30
1	A	862	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	A	862	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	626	GLY	N-CA-C	-7.23	95.02	113.10
1	A	460	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	52	ASN	C-N-CA	7.15	139.57	121.70
1	B	1010	PRO	CB-CA-C	-7.11	94.22	112.00
1	A	838	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	226	LEU	CB-CG-CD1	6.87	122.68	111.00
1	A	961	ARG	CB-CA-C	-6.65	97.10	110.40
1	A	759	LEU	CA-CB-CG	6.44	130.12	115.30
1	A	954	VAL	CB-CA-C	-6.39	99.25	111.40
2	C	17	LEU	CA-CB-CG	6.33	129.87	115.30
1	B	118	THR	N-CA-C	-6.23	94.17	111.00
1	A	67	LEU	CB-CG-CD1	-6.14	100.56	111.00
1	A	97	LEU	CB-CG-CD1	6.00	121.21	111.00
1	A	226	LEU	CA-CB-CG	5.98	129.06	115.30
1	B	626	GLY	C-N-CA	5.75	136.08	121.70
1	B	862	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	823	LEU	CB-CG-CD1	5.62	120.56	111.00
1	B	846	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	97	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	76	LEU	CB-CG-CD2	5.48	120.32	111.00
1	A	586	ASP	CB-CG-OD1	5.44	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	80	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	60	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	538	LEU	CA-CB-CG	-5.29	103.14	115.30
1	B	226	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	94	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	A	466	MET	CG-SD-CE	-5.22	91.85	100.20
1	B	455	LEU	CB-CA-C	5.21	120.10	110.20
1	A	577	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	A	867	LEU	CB-CG-CD1	5.11	119.68	111.00
1	B	892	ARG	NE-CZ-NH2	5.09	122.84	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	626	GLY	Peptide
1	B	119	LYS	Peptide
1	B	52	ASN	Peptide
1	B	626	GLY	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	7773	0	7633	114	0
1	B	7742	0	7600	114	0
2	C	78	0	74	2	0
2	D	82	0	78	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	124	0	0	2	0
4	B	110	0	0	2	0
All	All	15911	0	15385	227	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 7.

All (227) 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:623:THR:OG1	1:B:626:GLY:O	1.62	1.15
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.18	1.05
1:A:623:THR:OG1	1:A:626:GLY:O	1.75	1.03
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.11	0.98
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.50	0.92
1:B:309:ASP:H	1:B:672:ASN:HD21	1.18	0.90
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.35	0.90
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.02	0.89
1:A:294:GLN:H	1:A:297:HIS:HD2	1.21	0.88
1:A:309:ASP:H	1:A:672:ASN:HD21	1.21	0.86
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.74	0.85
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.80	0.81
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.00	0.79
1:B:102:ASN:H	1:B:102:ASN:HD22	1.28	0.78
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.63	0.78
1:A:229:ARG:CG	1:A:229:ARG:HH11	1.93	0.77
1:A:102:ASN:HD22	1:A:102:ASN:H	1.33	0.77
1:B:783:ASN:HD22	1:B:785:VAL:H	1.31	0.76
1:A:877:MET:O	1:A:933:LYS:NZ	2.18	0.76
1:A:491:ARG:NH1	1:A:491:ARG:HG3	1.95	0.76
1:B:119:LYS:O	1:B:119:LYS:HG2	1.86	0.75
1:A:771:LEU:HD21	1:A:954:VAL:HG22	1.69	0.74
1:B:125:ASN:H	1:B:125:ASN:HD22	1.36	0.74
1:A:622:ASN:H	1:A:622:ASN:HD22	1.35	0.74
1:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.35	0.73
1:B:960:ALA:HB3	1:B:963:MET:HG2	1.70	0.73
1:B:309:ASP:H	1:B:672:ASN:ND2	1.86	0.73
1:A:602:ASP:OD1	1:A:658:ARG:HD3	1.90	0.71
1:A:229:ARG:HG2	1:A:229:ARG:NH1	1.97	0.71
1:B:602:ASP:OD1	1:B:658:ARG:HD3	1.90	0.71
1:B:119:LYS:O	1:B:119:LYS:CG	2.39	0.70
1:B:603:SER:OG	1:B:648:LYS:HE3	1.92	0.70
1:A:222:ASN:O	1:A:226:LEU:HB2	1.91	0.69
1:A:329:ASN:HD22	1:A:332[B]:HIS:HB2	1.57	0.69
1:B:455:LEU:O	4:B:2063:HOH:O	2.10	0.69
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.41	0.68
1:A:309:ASP:H	1:A:672:ASN:ND2	1.91	0.68
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.77	0.68
1:A:782:ARG:NH1	1:A:963:MET:O	2.27	0.67
1:B:597:LEU:HD21	1:B:627:MET:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.95	0.67
1:B:294:GLN:H	1:B:297:HIS:HD2	1.43	0.66
1:A:783:ASN:ND2	1:A:786:HIS:H	1.94	0.66
1:A:196:ASN:HD22	1:A:199:TRP:H	1.45	0.64
1:A:294:GLN:H	1:A:297:HIS:CD2	2.10	0.64
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.45	0.64
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.78	0.64
1:B:783:ASN:ND2	1:B:785:VAL:H	1.96	0.64
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.79	0.63
1:B:730:HIS:HD2	1:B:904:SER:OG	1.82	0.63
1:A:329:ASN:ND2	1:A:332[B]:HIS:HD2	1.98	0.62
1:A:556:MET:HG3	1:A:556:MET:O	2.01	0.61
1:A:800:GLN:O	1:A:801:SER:HB3	2.00	0.61
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.30	0.61
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.81	0.61
1:A:329:ASN:ND2	1:A:332[B]:HIS:CD2	2.69	0.60
1:A:927:TYR:O	1:A:930:THR:HB	2.02	0.60
1:B:646:ILE:HD13	1:B:649:MET:HE3	1.82	0.60
1:A:386:HIS:HE1	4:A:2062:HOH:O	1.83	0.60
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.83	0.60
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.36	0.60
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.33	0.59
1:A:656:GLU:HB2	1:A:709:LEU:CD2	2.32	0.59
1:B:685:TYR:CZ	1:B:781:GLN:HG2	2.38	0.59
1:B:596:TYR:HE2	1:B:627:MET:HE1	1.68	0.59
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.85	0.59
1:A:413:GLU:HG2	1:A:531:ILE:HD11	1.83	0.59
1:B:600:LEU:HD21	1:B:648:LYS:HB3	1.86	0.58
1:B:927:TYR:O	1:B:930:THR:HB	2.04	0.58
1:A:125:ASN:HD22	1:A:125:ASN:H	1.52	0.58
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.86	0.57
1:B:596:TYR:HE2	1:B:627:MET:CE	2.17	0.57
1:A:299:LYS:HD2	1:A:510:ILE:HG13	1.86	0.57
1:B:783:ASN:ND2	1:B:786:HIS:H	2.03	0.56
1:B:102:ASN:N	1:B:102:ASN:HD22	2.02	0.56
1:A:102:ASN:HD22	1:A:102:ASN:N	2.02	0.56
1:A:860:GLU:OE2	1:A:957:HIS:HE1	1.88	0.56
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.52	0.56
1:A:860:GLU:OE2	1:A:957:HIS:CE1	2.58	0.55
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.87	0.55
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:THR:OG1	1:B:457:GLU:OE2	2.11	0.55
1:A:783:ASN:HD22	1:A:786:HIS:H	1.54	0.54
1:A:59:GLU:OE2	1:A:423:ARG:NH1	2.40	0.54
1:A:586:ASP:OD1	1:A:589:HIS:HD2	1.91	0.54
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.43	0.54
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.90	0.54
1:B:866:PHE:CZ	1:B:870:MET:HG2	2.44	0.53
1:A:843:ILE:HG22	1:A:844:GLN:H	1.74	0.53
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.91	0.52
1:B:184:ASN:HD21	1:B:223:LYS:HZ3	1.54	0.52
1:B:674:ARG:HD3	4:B:2085:HOH:O	2.09	0.52
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.45	0.52
1:B:602:ASP:OD1	1:B:658:ARG:CD	2.57	0.51
1:B:294:GLN:H	1:B:297:HIS:CD2	2.26	0.51
1:B:309:ASP:N	1:B:672:ASN:HD21	1.97	0.51
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.92	0.51
1:B:311:ARG:HA	1:B:481:VAL:O	2.11	0.50
1:B:184:ASN:ND2	1:B:223:LYS:NZ	2.52	0.50
1:A:843:ILE:HG22	1:A:844:GLN:N	2.26	0.50
1:B:646:ILE:HD13	1:B:649:MET:CE	2.41	0.50
1:A:622:ASN:H	1:A:622:ASN:ND2	2.06	0.50
1:A:329:ASN:HD21	1:A:332[B]:HIS:HD2	1.59	0.50
1:A:586:ASP:HB2	1:A:587:PRO:HD2	1.94	0.50
1:B:44:ASN:OD1	1:B:45:PRO:HD2	2.11	0.50
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.77	0.50
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.45	0.50
1:A:656:GLU:HB2	1:A:709:LEU:HD22	1.94	0.49
1:A:821:ASN:O	1:A:825:THR:HB	2.12	0.49
1:A:196:ASN:ND2	1:A:198:ALA:H	2.11	0.49
1:A:491:ARG:CG	1:A:491:ARG:HH11	2.10	0.49
1:B:597:LEU:HD11	1:B:627:MET:HE2	1.94	0.49
1:B:730:HIS:CD2	1:B:904:SER:OG	2.63	0.49
1:B:185:ALA:HB2	1:B:828:GLN:HE22	1.78	0.49
1:B:196:ASN:ND2	1:B:198:ALA:H	2.10	0.49
1:A:229:ARG:CG	1:A:229:ARG:NH1	2.66	0.49
1:A:771:LEU:HB2	1:A:796:GLN:OE1	2.12	0.49
1:A:303:LYS:HD3	1:A:485:PHE:CE2	2.48	0.49
1:A:329:ASN:HD21	1:A:332[B]:HIS:CD2	2.31	0.48
1:A:586:ASP:HB2	1:A:587:PRO:CD	2.43	0.47
1:B:102:ASN:H	1:B:102:ASN:ND2	2.04	0.47
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:C	1:B:67:LEU:HD12	2.35	0.47
1:A:67:LEU:C	1:A:67:LEU:HD12	2.35	0.47
1:A:44:ASN:HA	1:A:45:PRO:HD2	1.75	0.47
1:A:389:ASP:O	1:A:393:HIS:HD2	1.98	0.47
1:A:600:LEU:HD11	1:A:649:MET:CB	2.45	0.47
1:A:94:ILE:HD12	1:A:94:ILE:HG23	1.57	0.47
1:B:711:ARG:O	1:B:711:ARG:HG2	2.15	0.47
1:B:176:GLU:OE1	1:B:179:LYS:HE2	2.15	0.47
1:A:541:GLU:OE2	1:A:736:GLN:NE2	2.48	0.46
1:A:801:SER:O	1:A:802:THR:C	2.52	0.46
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.96	0.46
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.18	0.46
1:B:596:TYR:CE2	1:B:627:MET:CE	2.98	0.46
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.15	0.46
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.98	0.46
1:B:654:ILE:HD11	1:B:716:ILE:HD11	1.97	0.46
1:B:184:ASN:ND2	1:B:223:LYS:HZ2	2.10	0.46
1:B:466:MET:HB2	1:B:466:MET:HE3	1.50	0.45
1:B:136:GLY:CA	1:B:152:ASP:O	2.65	0.45
1:B:815:ILE:HG22	1:B:870:MET:HG3	1.98	0.45
1:B:685:TYR:OH	1:B:781:GLN:HG2	2.17	0.45
1:B:824:ARG:O	1:B:828:GLN:N	2.48	0.45
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.60	0.45
1:A:353:LYS:HD2	1:A:355:TRP:CZ3	2.52	0.45
1:A:595:LEU:O	1:A:599:LEU:HD12	2.17	0.45
1:B:597:LEU:HD11	1:B:627:MET:CE	2.47	0.44
1:A:824:ARG:O	1:A:828:GLN:HA	2.17	0.44
1:B:573:ASN:OD1	1:B:632:LYS:HG2	2.17	0.44
1:A:445:PRO:O	1:A:446:LEU:C	2.56	0.44
1:A:783:ASN:HD22	1:A:785:VAL:H	1.64	0.44
1:B:349:GLU:HA	1:B:349:GLU:OE2	2.18	0.44
1:B:852:SER:HB3	1:B:859:LEU:HD21	2.00	0.44
1:A:184:ASN:HD21	1:A:223:LYS:NZ	2.16	0.44
1:B:336:HIS:HD2	1:B:337:LEU:HD13	1.81	0.44
1:A:205:GLU:OE2	1:A:364:LYS:NZ	2.51	0.44
1:A:783:ASN:ND2	1:A:785:VAL:H	2.16	0.44
1:A:870:MET:O	1:A:874:ILE:HG13	2.17	0.44
1:B:881:ALA:O	1:B:884:LYS:HB2	2.18	0.43
1:B:824:ARG:O	1:B:828:GLN:HA	2.17	0.43
1:B:597:LEU:HA	1:B:597:LEU:HD12	1.80	0.43
1:B:196:ASN:ND2	1:B:198:ALA:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HG	1:B:75:VAL:HB	1.99	0.43
1:B:124:GLU:OE1	1:B:178:ALA:HB2	2.19	0.43
1:B:843:ILE:HG22	1:B:844:GLN:H	1.84	0.43
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.99	0.43
1:B:906:LYS:CE	1:B:921:ASP:OD2	2.66	0.43
1:B:771:LEU:HB3	1:B:952:HIS:HB3	2.00	0.43
1:A:805:ASN:HD22	1:A:844:GLN:NE2	2.13	0.43
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.80	0.43
1:B:359:LEU:HD23	1:B:359:LEU:C	2.39	0.43
1:A:220:THR:HG23	2:C:18:VAL:HG11	2.01	0.43
1:A:139:ASN:OD1	2:C:20:PHE:HB3	2.18	0.43
1:A:857:HIS:CD2	1:A:966:ASN:ND2	2.87	0.43
1:B:648:LYS:O	1:B:652:PHE:HB2	2.19	0.43
1:B:171:SER:HA	1:B:172:PRO:HD2	1.88	0.42
1:B:638:GLN:HB2	1:B:639:PRO:HD3	2.00	0.42
1:A:855:PRO:O	1:A:858:TYR:HB3	2.20	0.42
1:A:708:THR:HB	1:A:710:PRO:HD2	2.01	0.42
1:B:250:SER:O	1:B:254:MET:HG3	2.20	0.42
1:A:294:GLN:N	1:A:297:HIS:HD2	2.02	0.42
1:B:768:GLU:HB3	1:B:843:ILE:HG13	2.01	0.42
1:B:636:ASP:OD2	1:B:636:ASP:O	2.38	0.42
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.85	0.42
1:B:348:SER:OG	1:B:606:GLU:OE2	2.26	0.42
1:A:715:PHE:O	1:A:718:GLN:HB3	2.19	0.42
1:A:716:ILE:HB	1:A:717:PRO:HD3	2.01	0.42
1:B:708:THR:HB	1:B:710:PRO:HD2	2.02	0.42
1:A:810:LEU:HG	1:A:928:LEU:HD21	2.01	0.42
1:B:864:GLU:HG3	1:B:986:LEU:HD21	2.02	0.42
1:A:114:LEU:HD13	1:A:168:PHE:HB3	2.02	0.42
1:B:111:GLN:NE2	2:D:20:PHE:HB2	2.34	0.42
1:B:618:TYR:HA	1:B:630:SER:O	2.20	0.42
1:B:306:PRO:O	1:B:483:LYS:HE3	2.20	0.42
1:A:140:ALA:HA	1:A:148:ASN:O	2.19	0.41
1:A:197:ASP:O	1:A:201:LEU:HD22	2.20	0.41
1:A:75:VAL:HA	1:A:256:VAL:O	2.20	0.41
1:B:801:SER:O	1:B:802:THR:C	2.58	0.41
1:B:196:ASN:HD21	1:B:198:ALA:HB3	1.86	0.41
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.53	0.41
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.71	0.41
1:B:73:ILE:HG13	1:B:251:SER:HB2	2.00	0.41
1:A:450:LEU:HG	4:A:2072:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.55	0.41
1:B:846:LEU:HD13	1:B:848:PHE:CE1	2.56	0.41
1:B:683:MET:HA	1:B:792:GLU:OE2	2.21	0.41
1:A:759:LEU:O	1:A:760:PRO:C	2.59	0.41
1:A:491:ARG:CG	1:A:491:ARG:NH1	2.69	0.41
1:B:946:VAL:HA	1:B:951:ARG:CZ	2.51	0.41
1:B:136:GLY:HA3	1:B:152:ASP:O	2.21	0.41
1:B:118:THR:O	1:B:122:PRO:HA	2.21	0.41
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.56	0.41
1:A:345:SER:OG	1:A:348:SER:HB2	2.21	0.41
1:B:80:ASP:C	1:B:80:ASP:OD1	2.58	0.41
1:B:860:GLU:OE2	1:B:957:HIS:CE1	2.73	0.40
1:A:597:LEU:HD12	1:A:597:LEU:HA	1.85	0.40
1:B:586:ASP:OD1	1:B:589:HIS:HB2	2.21	0.40
1:B:86:SER:HB3	1:B:158:LEU:HG	2.03	0.40
1:A:723:LEU:HD12	1:A:755:THR:HG21	2.03	0.40
1:B:950:ARG:HD2	1:B:950:ARG:HH11	1.75	0.40
1:B:236:ASP:OD1	1:B:236:ASP:C	2.59	0.40
1:A:65:ARG:HB2	1:A:264:LEU:HD13	2.04	0.40
1:A:172:PRO:HG2	1:A:174:PHE:CE1	2.56	0.40
1:A:202:PHE:CZ	1:A:206:LYS:HE3	2.56	0.40
1:A:824:ARG:O	1:A:828:GLN:N	2.52	0.40
1:A:604:LEU:HA	1:A:604:LEU:HD23	1.93	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	955/1019 (94%)	920 (96%)	33 (4%)	2 (0%)	52 77
1	B	953/1019 (94%)	915 (96%)	37 (4%)	1 (0%)	56 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	6/42 (14%)	6 (100%)	0	0	100	100
2	D	6/42 (14%)	6 (100%)	0	0	100	100
All	All	1920/2122 (90%)	1847 (96%)	70 (4%)	3 (0%)	52	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	636	ASP
1	A	961	ARG
1	A	764	VAL

### 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	837/906 (92%)	760 (91%)	77 (9%)	11	21
1	B	831/906 (92%)	766 (92%)	65 (8%)	16	30
2	C	7/32 (22%)	5 (71%)	2 (29%)	0	1
2	D	8/32 (25%)	6 (75%)	2 (25%)	1	1
All	All	1683/1876 (90%)	1537 (91%)	146 (9%)	13	24

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	96	SER
1	A	97	LEU
1	A	102	ASN
1	A	125	ASN
1	A	158	LEU
1	A	177	SER
1	A	188	SER
1	A	196	ASN

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	226	LEU
1	A	229	ARG
1	A	243	LYS
1	A	270	LEU
1	A	281	LYS
1	A	285	LEU
1	A	329	ASN
1	A	332[A]	HIS
1	A	332[B]	HIS
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	412	GLN
1	A	417	LEU
1	A	423	ARG
1	A	431	ARG
1	A	446	LEU
1	A	450	LEU
1	A	455	LEU
1	A	466	MET
1	A	476	VAL
1	A	491	ARG
1	A	521	LYS
1	A	524	LEU
1	A	529	GLU
1	A	540	LEU
1	A	558	LYS
1	A	575	ASN
1	A	577	GLU
1	A	595	LEU
1	A	597	LEU
1	A	600	LEU
1	A	603	SER
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	653	GLU
1	A	655	ASP
1	A	656	GLU
1	A	677	GLN

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Mol	Chain	Res	Type
1	A	711	ARG
1	A	712	LEU
1	A	713	LYS
1	A	719	LEU
1	A	728	LEU
1	A	736	GLN
1	A	744	MET
1	A	771	LEU
1	A	784	GLU
1	A	810	LEU
1	A	817	GLU
1	A	823	LEU
1	A	846	LEU
1	A	859	LEU
1	A	860	GLU
1	A	867	LEU
1	A	871	GLU
1	A	873	SER
1	A	889	LEU
1	A	914	GLN
1	A	928	LEU
1	A	931	LEU
1	A	933	LYS
1	A	954	VAL
1	A	993	GLN
1	A	1007	LEU
1	B	76	LEU
1	B	94	ILE
1	B	97	LEU
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	154	SER
1	B	158	LEU
1	B	177	SER
1	B	196	ASN
1	B	201	LEU
1	B	226	LEU
1	B	270	LEU
1	B	281	LYS
1	B	285	LEU
1	B	337	LEU

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Mol	Chain	Res	Type
1	B	347	LEU
1	B	417	LEU
1	B	431	ARG
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	466	MET
1	B	470	LYS
1	B	482	SER
1	B	524	LEU
1	B	557	SER
1	B	595	LEU
1	B	597	LEU
1	B	600	LEU
1	B	603	SER
1	B	616	LEU
1	B	629	LEU
1	B	631	VAL
1	B	642	LEU
1	B	648	LYS
1	B	649	MET
1	B	677	GLN
1	B	712	LEU
1	B	719	LEU
1	B	728	LEU
1	B	744	MET
1	B	756	LYS
1	B	759	LEU
1	B	771	LEU
1	B	780	GLN
1	B	783	ASN
1	B	799	MET
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	838	ARG
1	B	846	LEU
1	B	854	LYS
1	B	859	LEU
1	B	867	LEU
1	B	870	MET
1	B	880	GLU

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Mol	Chain	Res	Type
1	B	889	LEU
1	B	892	ARG
1	B	898	LYS
1	B	928	LEU
1	B	941	LYS
1	B	1007	LEU
1	B	1011	HIS
2	C	17	LEU
2	C	18	VAL
2	D	17	LEU
2	D	18	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	129	GLN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	336	HIS
1	A	386	HIS
1	A	393	HIS
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	677	GLN
1	A	730	HIS
1	A	736	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	857	HIS
1	A	922	ASN

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Mol	Chain	Res	Type
1	A	957	HIS
1	A	966	ASN
1	B	93	HIS
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	184	ASN
1	B	196	ASN
1	B	297	HIS
1	B	300	GLN
1	B	386	HIS
1	B	393	HIS
1	B	407	GLN
1	B	502	GLN
1	B	605	ASN
1	B	672	ASN
1	B	677	GLN
1	B	680	GLN
1	B	730	HIS
1	B	780	GLN
1	B	783	ASN
1	B	805	ASN
1	B	821	ASN
1	B	828	GLN
1	B	883	GLN
1	B	922	ASN
1	B	957	HIS
1	B	979	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 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	958/1019 (94%)	-0.35	5 (0%) 91 90	20, 34, 52, 80	5 (0%)
1	B	956/1019 (93%)	-0.33	5 (0%) 91 90	24, 38, 54, 78	2 (0%)
2	C	10/42 (23%)	0.93	0 100 100	56, 73, 78, 79	0
2	D	10/42 (23%)	1.35	1 (10%) 9 6	64, 77, 82, 82	0
All	All	1934/2122 (91%)	-0.32	11 (0%) 90 88	20, 36, 54, 82	7 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332[A]	HIS	3.4
1	B	626	GLY	3.0
1	B	543	GLU	2.7
1	B	984	PRO	2.6
1	B	52	ASN	2.6
1	A	985	ALA	2.4
1	A	1012	ILE	2.3
2	D	21	ALA	2.2
1	A	626	GLY	2.2
1	B	544	ALA	2.1
1	A	517	ASP	2.1

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

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

### 6.3 Carbohydrates ⓘ

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
3	ZN	A	3013	1/1	0.98	0.11	-0.78	50,50,50,50	1
3	ZN	B	3013	1/1	0.97	0.07	-1.65	52,52,52,52	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.