



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 07:25 PM EDT

PDB ID : 3P7O  
Title : Rat Insulin Degrading Enzyme (Insulysin) E111F mutant with two bound peptides  
Authors : Rodgers, D.W.; Noinaj, N.  
Deposited on : unknown  
Resolution : 2.14 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

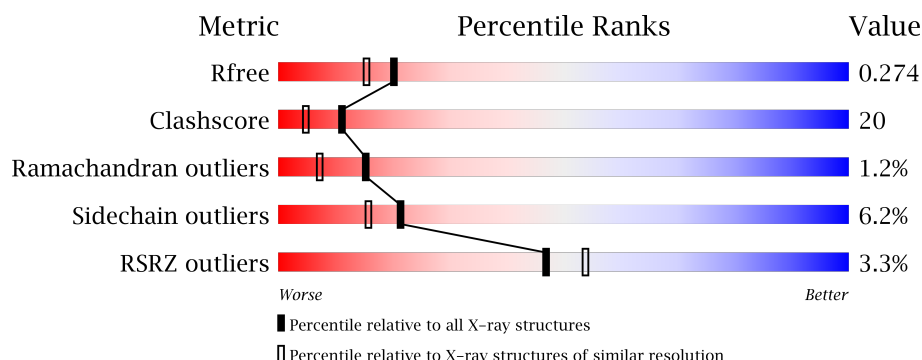
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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))
$R_{free}$	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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	<div> <div>3%</div> <div>58%</div> <div>33%</div> <div>6%</div> </div>
2	B	8	<div> <div>75%</div> <div>25%</div> </div>
3	C	7	<div> <div>71%</div> <div>29%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8094 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	31	0	0
			7834	5039	1318	1443	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	PHE	GLU	ENGINEERED MUTATION	UNP P35559

- Molecule 2 is a protein called active site bound peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			40	24	8	8			

- Molecule 3 is a protein called distal site bound peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			35	21	7	7			

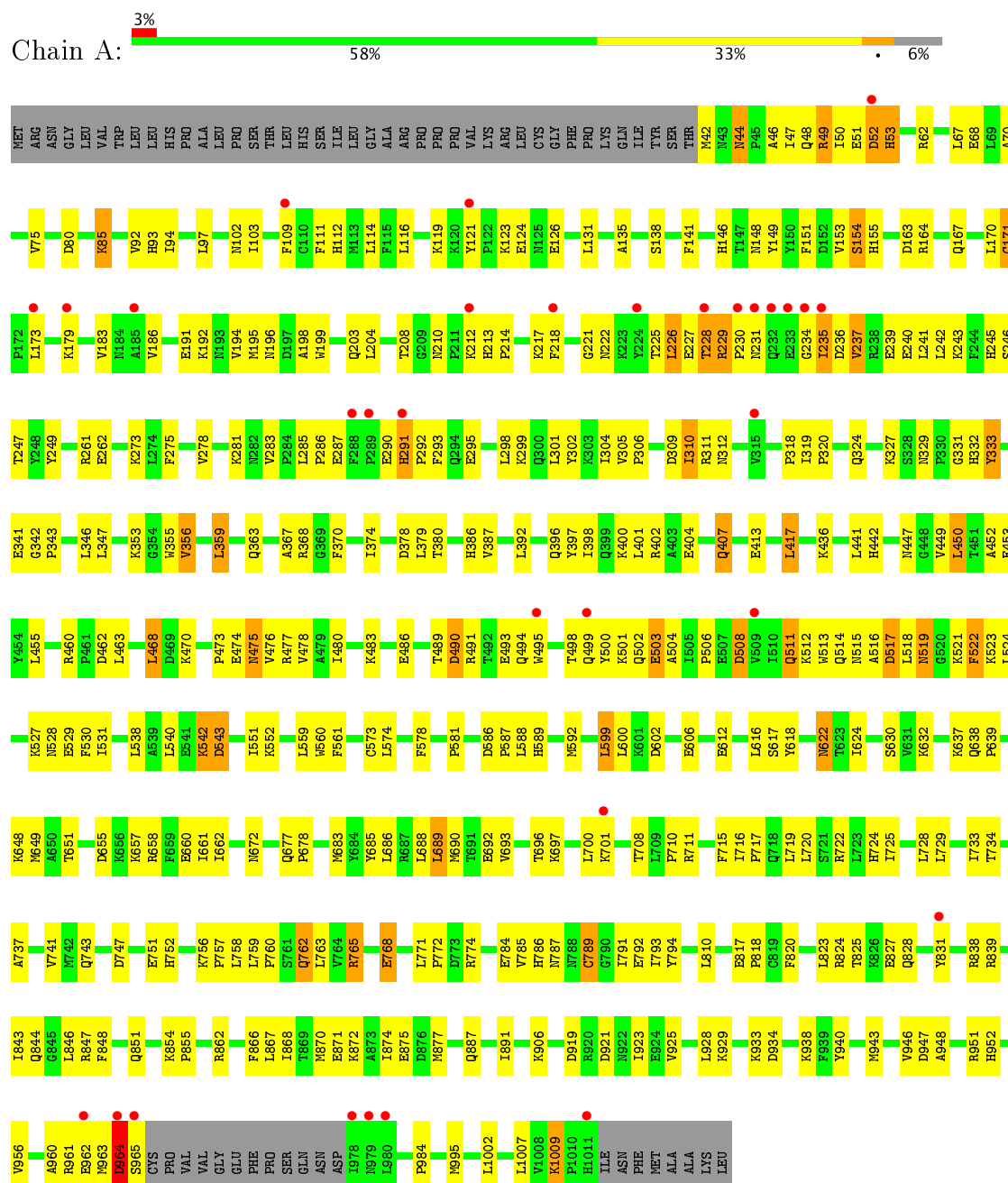
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total	O	0	0
			185	185		


### 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 2: active site bound peptide

Chain B:  75% 25%



- Molecule 3: distal site bound peptide

Chain C:  71% 29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.52Å 70.91Å 114.36Å 90.00° 92.97° 90.00°	Depositor
Resolution (Å)	28.84 – 2.14 28.84 – 2.14	Depositor EDS
% Data completeness (in resolution range)	92.7 (28.84-2.14) 92.7 (28.84-2.14)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.208 , 0.285 0.198 , 0.274	Depositor DCC
$R_{free}$ test set	4746 reflections (10.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.46	2/8032 (0.0%)	0.58	0/10865

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	768	GLU	CG-CD	7.78	1.63	1.51
1	A	768	GLU	CB-CG	7.52	1.66	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	7834	0	7755	312	0
2	B	40	0	11	3	0
3	C	35	0	10	1	0
4	A	185	0	0	10	0
All	All	8094	0	7776	313	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 20.

All (313) 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:817:GLU:HG3	1:A:818:PRO:HD3	1.32	1.09
1:A:51:GLU:HG2	1:A:53:HIS:H	1.22	0.99
1:A:44:ASN:ND2	1:A:46:ALA:H	1.61	0.98
1:A:1009:LYS:HE2	1:A:1009:LYS:H	1.27	0.95
1:A:44:ASN:HD22	1:A:46:ALA:H	1.09	0.94
1:A:963:MET:HG3	1:A:964:ASP:HB2	1.50	0.94
1:A:52:ASP:HB3	1:A:447:ASN:HB3	1.53	0.90
1:A:51:GLU:OE1	1:A:53:HIS:HA	1.71	0.89
1:A:490:ASP:HB2	1:A:491:ARG:HD2	1.51	0.89
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.58	0.85
1:A:689:LEU:HD13	1:A:995:MET:HG2	1.60	0.83
1:A:51:GLU:HG2	1:A:53:HIS:N	1.93	0.82
1:A:760:PRO:HA	1:A:763:LEU:HD12	1.59	0.81
1:A:51:GLU:O	1:A:52:ASP:HB2	1.79	0.81
1:A:490:ASP:HB2	1:A:491:ARG:HH21	1.46	0.80
1:A:196:ASN:HD22	1:A:199:TRP:H	1.33	0.76
1:A:234:GLY:O	1:A:235:ILE:HB	1.85	0.76
1:A:728:LEU:O	1:A:729:LEU:HD23	1.87	0.75
1:A:324:GLN:HG2	4:A:1081:HOH:O	1.86	0.75
1:A:887:GLN:HB2	4:A:1175:HOH:O	1.87	0.74
1:A:658:ARG:HH21	1:A:661:ILE:HD12	1.52	0.74
1:A:491:ARG:NH2	1:A:501:LYS:HD2	2.03	0.74
1:A:183:VAL:HG21	1:A:227:GLU:HG3	1.67	0.74
1:A:963:MET:CG	1:A:964:ASP:HB2	2.18	0.74
1:A:1009:LYS:HE2	1:A:1009:LYS:N	2.01	0.73
1:A:342:GLY:HA2	1:A:606:GLU:CG	2.20	0.72
1:A:51:GLU:CG	1:A:53:HIS:H	2.03	0.71
1:A:404:GLU:HG3	1:A:407:GLN:HE22	1.56	0.70
1:A:961:ARG:HD2	1:A:962:GLU:OE2	1.92	0.70
1:A:342:GLY:HA2	1:A:606:GLU:HG2	1.74	0.69
1:A:689:LEU:HB3	1:A:690:MET:HE3	1.74	0.69
1:A:651:THR:HA	4:A:1184:HOH:O	1.91	0.69
1:A:141:PHE:CE1	1:A:148:ASN:HB3	2.28	0.69
1:A:109:PHE:CD1	1:A:226:LEU:HG	2.27	0.69
1:A:285:LEU:HD12	1:A:286:PRO:HD2	1.75	0.69
1:A:291:HIS:NE2	1:A:318:PRO:HB3	2.07	0.69
1:A:356:VAL:HG22	1:A:378:ASP:O	1.93	0.68
1:A:222:ASN:O	1:A:226:LEU:HB2	1.93	0.68
1:A:48:GLN:HG3	1:A:70:ALA:HA	1.75	0.68
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.74	0.68
1:A:196:ASN:ND2	1:A:199:TRP:H	1.91	0.67
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASN:OD1	1:A:212:LYS:HG2	1.95	0.66
1:A:499:GLN:O	1:A:500:TYR:HB3	1.94	0.66
1:A:387:VAL:HG11	1:A:480:ILE:HD11	1.76	0.65
1:A:155:HIS:CD2	1:A:261:ARG:HD2	2.31	0.65
1:A:44:ASN:HD22	1:A:46:ALA:N	1.89	0.65
1:A:964:ASP:O	1:A:965:SER:HB3	1.95	0.65
1:A:245:HIS:O	1:A:249:TYR:HB2	1.97	0.65
1:A:309:ASP:H	1:A:672:ASN:ND2	1.94	0.64
1:A:331:GLY:HA3	1:A:363:GLN:OE1	1.97	0.64
1:A:146:HIS:HE1	1:A:442:HIS:HD2	1.45	0.64
1:A:291:HIS:HE1	1:A:293:PHE:HB2	1.63	0.64
1:A:871:GLU:HG3	1:A:940:TYR:CE1	2.33	0.64
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.78	0.64
1:A:196:ASN:HD21	1:A:198:ALA:HB3	1.61	0.63
1:A:51:GLU:HG2	1:A:52:ASP:N	2.13	0.63
1:A:109:PHE:HE1	1:A:183:VAL:HG22	1.63	0.63
1:A:658:ARG:O	1:A:662:ILE:HG12	1.97	0.63
1:A:213:HIS:ND1	1:A:214:PRO:HD2	2.14	0.62
1:A:823:LEU:HD11	1:A:866:PHE:HB2	1.81	0.62
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.81	0.61
1:A:490:ASP:CB	1:A:491:ARG:HH21	2.11	0.61
1:A:696:THR:O	1:A:700:LEU:HD22	2.01	0.61
1:A:586:ASP:OD1	1:A:589:HIS:HD2	1.84	0.61
1:A:333:TYR:CD2	1:A:333:TYR:C	2.75	0.60
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.83	0.60
1:A:600:LEU:HD21	1:A:649:MET:HG3	1.81	0.60
1:A:728:LEU:C	1:A:729:LEU:HD23	2.21	0.60
1:A:831:TYR:HE1	2:B:12:UNK:CB	2.13	0.60
1:A:309:ASP:H	1:A:672:ASN:HD21	1.50	0.59
1:A:154:SER:HB2	1:A:891:ILE:HD13	1.83	0.59
1:A:228:THR:HG22	1:A:229:ARG:N	2.15	0.59
1:A:246:SER:O	1:A:281:LYS:HD3	2.02	0.59
1:A:470:LYS:HE3	1:A:475:ASN:ND2	2.18	0.59
1:A:332:HIS:CE1	1:A:363:GLN:HG2	2.37	0.59
1:A:490:ASP:HB2	1:A:491:ARG:NH2	2.16	0.58
1:A:291:HIS:CE1	1:A:293:PHE:HB2	2.39	0.57
1:A:542:LYS:CD	1:A:542:LYS:H	2.17	0.57
1:A:237:VAL:O	1:A:241:LEU:HG	2.04	0.57
1:A:319:ILE:HB	1:A:320:PRO:HD2	1.87	0.56
1:A:208:THR:OG1	1:A:302:TYR:CZ	2.56	0.56
1:A:491:ARG:NH1	1:A:502:GLN:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:THR:HG22	1:A:499:GLN:O	2.05	0.56
1:A:50:ILE:HG12	1:A:67:LEU:CD2	2.35	0.56
1:A:787:ASN:ND2	1:A:961:ARG:CZ	2.68	0.56
1:A:751:GLU:HG3	1:A:752:HIS:CD2	2.40	0.56
1:A:831:TYR:CE1	2:B:12:UNK:CB	2.89	0.55
1:A:295:GLU:HA	1:A:298:LEU:HD12	1.88	0.55
1:A:342:GLY:HA3	1:A:606:GLU:HA	1.88	0.55
1:A:374:ILE:HD12	1:A:374:ILE:O	2.07	0.55
1:A:52:ASP:CB	1:A:447:ASN:HB3	2.33	0.55
1:A:503:GLU:HG3	1:A:504:ALA:N	2.20	0.55
1:A:234:GLY:O	1:A:235:ILE:CB	2.55	0.54
1:A:387:VAL:HG21	1:A:480:ILE:HD13	1.89	0.54
1:A:306:PRO:HG2	1:A:483:LYS:CD	2.37	0.54
1:A:578:PHE:CD2	1:A:725:ILE:HG12	2.43	0.54
1:A:508:ASP:HA	1:A:511:GLN:HB2	1.90	0.53
1:A:367:ALA:HB3	1:A:370:PHE:CE2	2.43	0.53
1:A:153:VAL:HG22	1:A:154:SER:N	2.22	0.53
1:A:374:ILE:HD12	1:A:374:ILE:C	2.28	0.53
1:A:810:LEU:O	1:A:810:LEU:HD12	2.08	0.53
1:A:504:ALA:O	1:A:506:PRO:HD3	2.08	0.53
1:A:170:LEU:O	1:A:171:CYS:HB3	2.09	0.53
1:A:561:PHE:HE1	1:A:733:ILE:HG13	1.73	0.53
1:A:586:ASP:HB2	1:A:587:PRO:HD2	1.89	0.53
1:A:229:ARG:N	1:A:230:PRO:CD	2.72	0.53
1:A:301:LEU:HD12	1:A:302:TYR:N	2.25	0.52
1:A:524:LEU:HB2	4:A:1074:HOH:O	2.08	0.52
1:A:622:ASN:H	1:A:622:ASN:HD22	1.56	0.52
1:A:638:GLN:N	1:A:639:PRO:CD	2.72	0.52
1:A:825:THR:C	1:A:828:GLN:NE2	2.63	0.52
1:A:240:GLU:OE1	1:A:240:GLU:HA	2.09	0.52
1:A:392:LEU:O	1:A:396:GLN:HG3	2.09	0.52
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.09	0.52
1:A:871:GLU:O	1:A:875:GLU:HG3	2.08	0.52
1:A:470:LYS:HE3	1:A:475:ASN:HD21	1.75	0.52
1:A:612:GLU:OE1	1:A:617:SER:HB3	2.10	0.52
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.90	0.52
1:A:793:ILE:O	1:A:847:ARG:HA	2.10	0.52
1:A:785:VAL:HG12	1:A:786:HIS:CD2	2.44	0.52
1:A:146:HIS:CE1	1:A:442:HIS:HD2	2.27	0.52
1:A:616:LEU:HD12	1:A:632:LYS:O	2.09	0.52
1:A:112:HIS:CD2	1:A:186:VAL:HG22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:O	1:A:291:HIS:HB3	2.10	0.52
1:A:301:LEU:HD13	1:A:478:VAL:HG23	1.91	0.51
1:A:960:ALA:O	1:A:963:MET:O	2.28	0.51
1:A:722:ARG:HG2	1:A:756:LYS:HG3	1.92	0.51
1:A:678:PRO:HD2	1:A:851:GLN:OE1	2.11	0.51
1:A:514:GLN:C	1:A:516:ALA:H	2.14	0.51
1:A:586:ASP:HB2	1:A:587:PRO:CD	2.41	0.51
1:A:247:THR:O	1:A:283:VAL:HG21	2.11	0.51
1:A:820:PHE:CE1	1:A:824:ARG:HD3	2.45	0.51
1:A:581:PRO:HD3	1:A:758:LEU:HD21	1.92	0.51
1:A:759:LEU:O	1:A:762:GLN:HG2	2.11	0.51
1:A:163:ASP:O	1:A:167:GLN:HG2	2.11	0.50
1:A:121:TYR:HB3	1:A:126:GLU:HG2	1.92	0.50
1:A:574:LEU:HD21	1:A:638:GLN:OE1	2.11	0.50
1:A:838:ARG:C	1:A:839:ARG:HD2	2.31	0.50
1:A:441:LEU:CD2	1:A:449:VAL:HG11	2.40	0.50
1:A:49:ARG:HG2	1:A:68:GLU:HB3	1.92	0.50
1:A:306:PRO:HG2	1:A:483:LYS:HD3	1.93	0.49
1:A:489:THR:HB	1:A:500:TYR:H	1.76	0.49
1:A:559:LEU:HD12	1:A:560:TRP:N	2.27	0.49
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.94	0.49
1:A:493:GLU:OE2	1:A:495:TRP:HD1	1.95	0.49
1:A:67:LEU:HB2	1:A:75:VAL:HB	1.93	0.49
1:A:236:ASP:O	1:A:240:GLU:HG2	2.13	0.49
1:A:203:GLN:HG3	1:A:203:GLN:O	2.13	0.49
1:A:452:ALA:O	1:A:453:GLU:HB2	2.13	0.49
1:A:768:GLU:HB3	1:A:843:ILE:HG13	1.95	0.49
1:A:948:ALA:HB3	1:A:951:ARG:HB2	1.94	0.49
1:A:305:VAL:HG21	1:A:486:GLU:HA	1.95	0.49
1:A:697:LYS:O	1:A:701:LYS:HG3	2.13	0.49
1:A:688:LEU:CD1	1:A:696:THR:HG22	2.38	0.48
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.93	0.48
1:A:413:GLU:OE2	1:A:527:LYS:HE2	2.13	0.48
1:A:225:THR:HG21	1:A:495:TRP:HZ3	1.79	0.48
1:A:854:LYS:HB3	1:A:855:PRO:HD2	1.95	0.48
1:A:402:ARG:HG2	1:A:468:LEU:HD13	1.94	0.48
1:A:934:ASP:O	1:A:938:LYS:HG3	2.13	0.48
1:A:109:PHE:CE1	1:A:226:LEU:HG	2.48	0.48
1:A:191:GLU:HA	1:A:194:VAL:HG23	1.95	0.48
1:A:109:PHE:CE2	1:A:241:LEU:HD11	2.47	0.48
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASN:OD1	1:A:519:ASN:C	2.52	0.48
1:A:131:LEU:CD1	1:A:138:SER:HB3	2.44	0.48
1:A:51:GLU:HG2	1:A:52:ASP:H	1.77	0.48
1:A:622:ASN:H	1:A:622:ASN:ND2	2.12	0.48
1:A:685:TYR:HB2	1:A:956:VAL:HG11	1.95	0.48
1:A:1009:LYS:CE	1:A:1009:LYS:H	2.13	0.48
3:C:6:UNK:O	3:C:7:UNK:CB	2.61	0.48
1:A:179:LYS:CE	1:A:237:VAL:HG23	2.43	0.48
1:A:342:GLY:CA	1:A:606:GLU:HA	2.44	0.48
1:A:398:ILE:O	1:A:401:LEU:N	2.46	0.48
1:A:62:ARG:HG2	1:A:80:ASP:HB2	1.95	0.47
1:A:715:PHE:CZ	1:A:719:LEU:HD22	2.48	0.47
1:A:827:GLU:OE1	1:A:862:ARG:HD3	2.13	0.47
1:A:490:ASP:CG	1:A:491:ARG:NH2	2.68	0.47
1:A:763:LEU:HB2	4:A:1124:HOH:O	2.13	0.47
1:A:229:ARG:N	1:A:230:PRO:HD2	2.30	0.47
1:A:243:LYS:O	1:A:247:THR:HG23	2.14	0.47
1:A:529:GLU:HA	1:A:529:GLU:OE2	2.15	0.47
1:A:960:ALA:HB3	1:A:963:MET:HB3	1.96	0.47
1:A:765:ARG:NH1	4:A:1130:HOH:O	2.48	0.47
1:A:109:PHE:HE2	1:A:241:LEU:HD11	1.79	0.46
1:A:230:PRO:O	1:A:234:GLY:O	2.32	0.46
1:A:491:ARG:HB2	1:A:500:TYR:CE1	2.50	0.46
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.81	0.46
1:A:214:PRO:HA	1:A:217:LYS:HE2	1.97	0.46
1:A:51:GLU:CG	1:A:52:ASP:N	2.77	0.46
1:A:919:ASP:O	1:A:923:ILE:HG13	2.16	0.46
1:A:513:TRP:O	1:A:516:ALA:HB2	2.15	0.46
1:A:309:ASP:N	1:A:672:ASN:HD21	2.14	0.46
1:A:772:PRO:HD3	1:A:1002:LEU:HD22	1.97	0.46
1:A:353:LYS:HA	1:A:353:LYS:HE2	1.97	0.46
1:A:103:ILE:HD11	1:A:240:GLU:HG3	1.98	0.46
1:A:686:LEU:HD22	1:A:792:GLU:HG2	1.97	0.46
1:A:689:LEU:CD1	1:A:995:MET:HG2	2.40	0.46
1:A:291:HIS:CD2	1:A:292:PRO:HD2	2.50	0.46
1:A:508:ASP:OD1	1:A:508:ASP:N	2.49	0.46
1:A:573:CYS:C	1:A:574:LEU:HD23	2.36	0.46
1:A:683:MET:HA	1:A:792:GLU:OE2	2.16	0.46
1:A:708:THR:OG1	1:A:710:PRO:HD2	2.16	0.46
1:A:493:GLU:OE2	1:A:495:TRP:CD1	2.69	0.45
1:A:542:LYS:H	1:A:542:LYS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:LEU:HD22	1:A:1007:LEU:N	2.31	0.45
1:A:246:SER:O	1:A:281:LYS:CD	2.65	0.45
1:A:291:HIS:HA	1:A:292:PRO:HD3	1.72	0.45
1:A:473:PRO:O	1:A:476:VAL:HG12	2.17	0.45
1:A:47:ILE:HG21	1:A:50:ILE:HG13	1.99	0.45
1:A:677:GLN:NE2	1:A:786:HIS:HE1	2.14	0.45
1:A:843:ILE:HG22	1:A:844:GLN:N	2.32	0.45
1:A:275:PHE:O	1:A:278:VAL:HG23	2.17	0.45
1:A:586:ASP:OD1	1:A:589:HIS:CD2	2.67	0.45
1:A:963:MET:CB	1:A:964:ASP:HB2	2.47	0.45
1:A:491:ARG:CD	1:A:491:ARG:N	2.80	0.45
1:A:102:ASN:N	1:A:102:ASN:OD1	2.50	0.45
1:A:964:ASP:HB3	1:A:965:SER:H	1.51	0.44
1:A:195:MET:HE2	1:A:195:MET:HA	1.99	0.44
1:A:724:HIS:CE1	1:A:760:PRO:HG3	2.53	0.44
1:A:460:ARG:CB	1:A:463:LEU:HD12	2.47	0.44
1:A:517:ASP:O	1:A:518:LEU:HD12	2.18	0.44
1:A:789:CYS:HB3	1:A:963:MET:SD	2.58	0.44
1:A:123:LYS:HB3	1:A:126:GLU:HB2	2.00	0.44
1:A:508:ASP:O	1:A:512:LYS:N	2.49	0.44
1:A:762:GLN:HE21	1:A:762:GLN:HB3	1.69	0.44
1:A:92:VAL:HG12	1:A:94:ILE:H	1.83	0.44
1:A:346:LEU:HA	1:A:522:PHE:CE2	2.53	0.43
1:A:530:PHE:HA	1:A:637:LYS:HD3	1.99	0.43
1:A:455:LEU:HA	4:A:1146:HOH:O	2.17	0.43
1:A:925:VAL:O	1:A:929:LYS:HG3	2.18	0.43
1:A:574:LEU:N	1:A:574:LEU:HD23	2.33	0.43
1:A:655:ASP:OD1	1:A:657:LYS:N	2.51	0.43
1:A:870:MET:HA	1:A:870:MET:CE	2.49	0.43
1:A:44:ASN:ND2	1:A:44:ASN:C	2.72	0.43
1:A:387:VAL:HG21	1:A:480:ILE:CD1	2.48	0.43
1:A:686:LEU:HD21	1:A:794:TYR:HB2	2.00	0.43
1:A:218:PHE:CE2	1:A:221:GLY:N	2.86	0.43
1:A:588:LEU:O	1:A:592:MET:HG3	2.18	0.43
1:A:756:LYS:HB3	1:A:756:LYS:HE2	1.80	0.43
1:A:204:LEU:CD2	1:A:304:ILE:HG12	2.49	0.43
1:A:126:GLU:OE1	1:A:164:ARG:NE	2.35	0.43
1:A:301:LEU:HD12	1:A:302:TYR:H	1.83	0.43
1:A:310:ILE:HB	1:A:312:ASN:ND2	2.34	0.43
1:A:397:TYR:O	1:A:400:LYS:HB3	2.19	0.43
1:A:436:LYS:HD2	1:A:436:LYS:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:THR:HG21	1:A:499:GLN:HB3	2.00	0.42
1:A:827:GLU:O	1:A:828:GLN:C	2.58	0.42
1:A:359:LEU:CD1	1:A:359:LEU:C	2.87	0.42
1:A:417:LEU:HA	1:A:417:LEU:HD12	1.90	0.42
1:A:521:LYS:O	1:A:523:LYS:HG2	2.19	0.42
1:A:236:ASP:HB3	1:A:239:GLU:CB	2.49	0.42
1:A:44:ASN:HD22	1:A:44:ASN:C	2.23	0.42
1:A:868:ILE:HD11	1:A:984:PRO:HG3	2.02	0.42
1:A:170:LEU:O	1:A:171:CYS:CB	2.67	0.42
1:A:791:ILE:HD11	1:A:793:ILE:HD11	2.01	0.42
1:A:291:HIS:CE1	1:A:293:PHE:H	2.37	0.42
1:A:51:GLU:OE1	1:A:53:HIS:CA	2.55	0.42
1:A:774:ARG:HD3	4:A:1099:HOH:O	2.19	0.42
1:A:825:THR:O	1:A:828:GLN:NE2	2.52	0.42
1:A:208:THR:HG21	1:A:477:ARG:HH12	1.85	0.42
1:A:551:ILE:HD13	1:A:561:PHE:HB3	2.01	0.42
1:A:868:ILE:O	1:A:872:LYS:HG3	2.20	0.42
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.72	0.42
1:A:85:LYS:HE3	1:A:135:ALA:O	2.20	0.42
1:A:93:HIS:HE1	1:A:368:ARG:HE	1.68	0.42
1:A:355:TRP:C	1:A:380:THR:HG23	2.41	0.42
1:A:756:LYS:HB2	1:A:757:PRO:CD	2.50	0.42
1:A:839:ARG:NH1	4:A:1168:HOH:O	2.42	0.42
1:A:151:PHE:C	1:A:151:PHE:CD1	2.93	0.41
1:A:341:GLU:HG2	1:A:347:LEU:HD23	2.01	0.41
1:A:528:ASN:OD1	1:A:531:ILE:HG13	2.19	0.41
1:A:772:PRO:HD3	1:A:1002:LEU:CD2	2.50	0.41
1:A:225:THR:HG21	1:A:495:TRP:CZ3	2.55	0.41
1:A:737:ALA:O	1:A:741:VAL:HG23	2.20	0.41
1:A:874:ILE:O	1:A:933:LYS:HE3	2.20	0.41
1:A:199:TRP:CZ2	2:B:8:UNK:HA	2.54	0.41
1:A:286:PRO:O	1:A:287:GLU:HG3	2.20	0.41
1:A:311:ARG:HB3	1:A:379:LEU:HB2	2.02	0.41
1:A:785:VAL:HB	1:A:786:HIS:HD2	1.86	0.41
1:A:355:TRP:HZ2	1:A:386:HIS:CD2	2.39	0.41
1:A:618:TYR:HA	1:A:630:SER:O	2.19	0.41
1:A:146:HIS:HE1	1:A:442:HIS:CD2	2.31	0.41
1:A:179:LYS:HE3	1:A:237:VAL:HG23	2.02	0.41
1:A:542:LYS:HD3	1:A:543:ASP:OD1	2.21	0.41
1:A:599:LEU:HD13	1:A:599:LEU:HA	1.95	0.41
1:A:660:GLU:HB2	4:A:1031:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:LEU:HD21	1:A:848:PHE:HE1	1.86	0.41
1:A:119:LYS:HA	1:A:173:LEU:HD21	2.03	0.41
1:A:846:LEU:HD12	1:A:847:ARG:N	2.36	0.41
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.89	0.41
1:A:183:VAL:HG21	1:A:227:GLU:CG	2.43	0.41
1:A:825:THR:C	1:A:828:GLN:HE22	2.24	0.41
1:A:747:ASP:O	1:A:751:GLU:HG2	2.19	0.41
1:A:114:LEU:HD12	1:A:149:TYR:OH	2.21	0.41
1:A:309:ASP:HB3	1:A:672:ASN:HD21	1.85	0.41
1:A:491:ARG:HD2	1:A:491:ARG:N	2.36	0.40
1:A:213:HIS:ND1	1:A:214:PRO:CD	2.82	0.40
1:A:246:SER:HA	1:A:281:LYS:HE3	2.03	0.40
1:A:690:MET:CE	1:A:690:MET:HA	2.51	0.40
1:A:285:LEU:HD12	1:A:286:PRO:CD	2.49	0.40
1:A:332:HIS:NE2	1:A:363:GLN:HG2	2.37	0.40
1:A:490:ASP:CG	1:A:491:ARG:HH21	2.24	0.40
1:A:116:LEU:HD22	1:A:124:GLU:HG3	2.03	0.40
1:A:612:GLU:CD	1:A:617:SER:HB3	2.42	0.40
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.51	0.40
1:A:109:PHE:CD2	1:A:241:LEU:HD21	2.56	0.40
1:A:242:LEU:HA	1:A:242:LEU:HD23	1.83	0.40
1:A:299:LYS:HD3	1:A:474:GLU:HA	2.04	0.40
1:A:715:PHE:CE2	1:A:719:LEU:HD22	2.56	0.40
1:A:921:ASP:O	1:A:925:VAL:HG23	2.22	0.40
1:A:94:ILE:HD12	1:A:94:ILE:HA	1.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	954/1019 (94%)	891 (93%)	52 (6%)	11 (1%)	15 7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	964	ASP
1	A	235	ILE
1	A	517	ASP
1	A	53	HIS
1	A	522	PHE
1	A	291	HIS
1	A	171	CYS
1	A	343	PRO
1	A	515	ASN
1	A	262	GLU

### 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	857/910 (94%)	804 (94%)	53 (6%)	21	16

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	MET
1	A	44	ASN
1	A	49	ARG
1	A	85	LYS
1	A	111	PHE
1	A	154	SER
1	A	192	LYS
1	A	226	LEU
1	A	228	THR
1	A	229	ARG
1	A	231	ASN
1	A	237	VAL
1	A	273	LYS
1	A	310	ILE

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Mol	Chain	Res	Type
1	A	327	LYS
1	A	329	ASN
1	A	333	TYR
1	A	356	VAL
1	A	359	LEU
1	A	407	GLN
1	A	417	LEU
1	A	450	LEU
1	A	462	ASP
1	A	468	LEU
1	A	475	ASN
1	A	490	ASP
1	A	494	GLN
1	A	503	GLU
1	A	508	ASP
1	A	511	GLN
1	A	519	ASN
1	A	542	LYS
1	A	543	ASP
1	A	599	LEU
1	A	622	ASN
1	A	624	ILE
1	A	648	LYS
1	A	689	LEU
1	A	711	ARG
1	A	720	LEU
1	A	743	GLN
1	A	762	GLN
1	A	765	ARG
1	A	784	GLU
1	A	789	CYS
1	A	867	LEU
1	A	877	MET
1	A	928	LEU
1	A	943	MET
1	A	946	VAL
1	A	947	ASP
1	A	964	ASP
1	A	1009	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	93	HIS
1	A	108	HIS
1	A	112	HIS
1	A	155	HIS
1	A	157	HIS
1	A	190	HIS
1	A	196	ASN
1	A	232	GLN
1	A	294	GLN
1	A	300	GLN
1	A	312	ASN
1	A	407	GLN
1	A	442	HIS
1	A	502	GLN
1	A	511	GLN
1	A	575	ASN
1	A	589	HIS
1	A	622	ASN
1	A	672	ASN
1	A	724	HIS
1	A	752	HIS
1	A	762	GLN
1	A	786	HIS
1	A	787	ASN
1	A	828	GLN
1	A	857	HIS
1	A	883	GLN
1	A	887	GLN

### 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 [i](#)

There are no ligands in this entry.

## 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	958/1019 (94%)	0.19	32 (3%) 47 54	21, 45, 75, 108	7 (0%)
2	B	0/8	-	-	-	-
3	C	0/7	-	-	-	-
All	All	958/1034 (92%)	0.19	32 (3%) 47 54	21, 45, 75, 108	7 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	979	ASN	5.5
1	A	978	ILE	4.7
1	A	212	LYS	4.7
1	A	228	THR	4.5
1	A	179	LYS	4.4
1	A	289	PRO	3.9
1	A	231	ASN	3.9
1	A	235	ILE	3.5
1	A	52	ASP	3.5
1	A	980	LEU	3.4
1	A	291	HIS	3.3
1	A	962	GLU	3.2
1	A	109	PHE	3.1
1	A	234	GLY	3.0
1	A	224	TYR	3.0
1	A	185	ALA	2.9
1	A	964	ASP	2.8
1	A	230	PRO	2.8
1	A	509	VAL	2.6
1	A	218	PHE	2.5
1	A	495	TRP	2.5
1	A	233	GLU	2.4
1	A	288	PHE	2.3
1	A	315	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	965	SER	2.3
1	A	831	TYR	2.3
1	A	1011	HIS	2.3
1	A	701	LYS	2.2
1	A	173	LEU	2.2
1	A	121	TYR	2.1
1	A	499	GLN	2.0
1	A	232	GLN	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.