



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:11 AM GMT

PDB ID : 3HGZ  
Title : Crystal structure of human insulin-degrading enzyme in complex with amylin  
Authors : Guo, Q.; Bian, Y.; Tang, W.J.  
Deposited on : 2009-05-14  
Resolution : 2.91 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

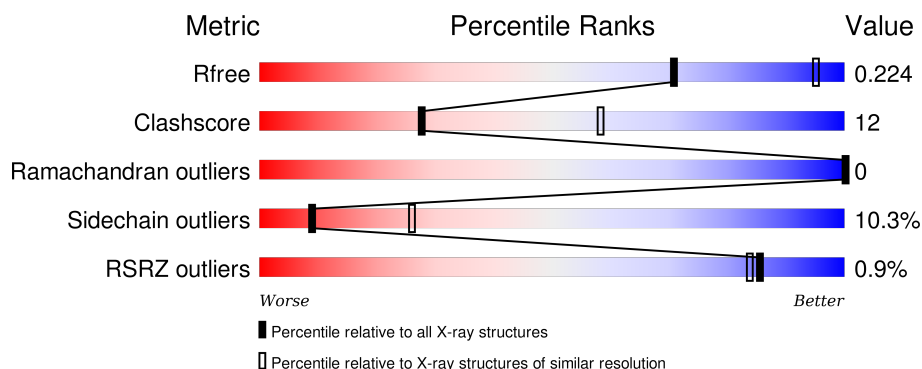
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	969	 73% 22% . .
1	B	969	 70% 25% . .
2	D	37	 3% 14% 81%
2	E	37	 11% 11% 8% 5% 73%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16156 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	0
			7837	5045	1317	1453	22			
1	B	959	Total	C	N	O	S	0	0	0
			7844	5050	1318	1454	22			

There are 28 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called Islet amyloid polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	S	0	0	0
			55	37	9	8	1			
2	E	10	Total	C	N	O	S	0	0	0
			71	46	12	11	2			

- 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		

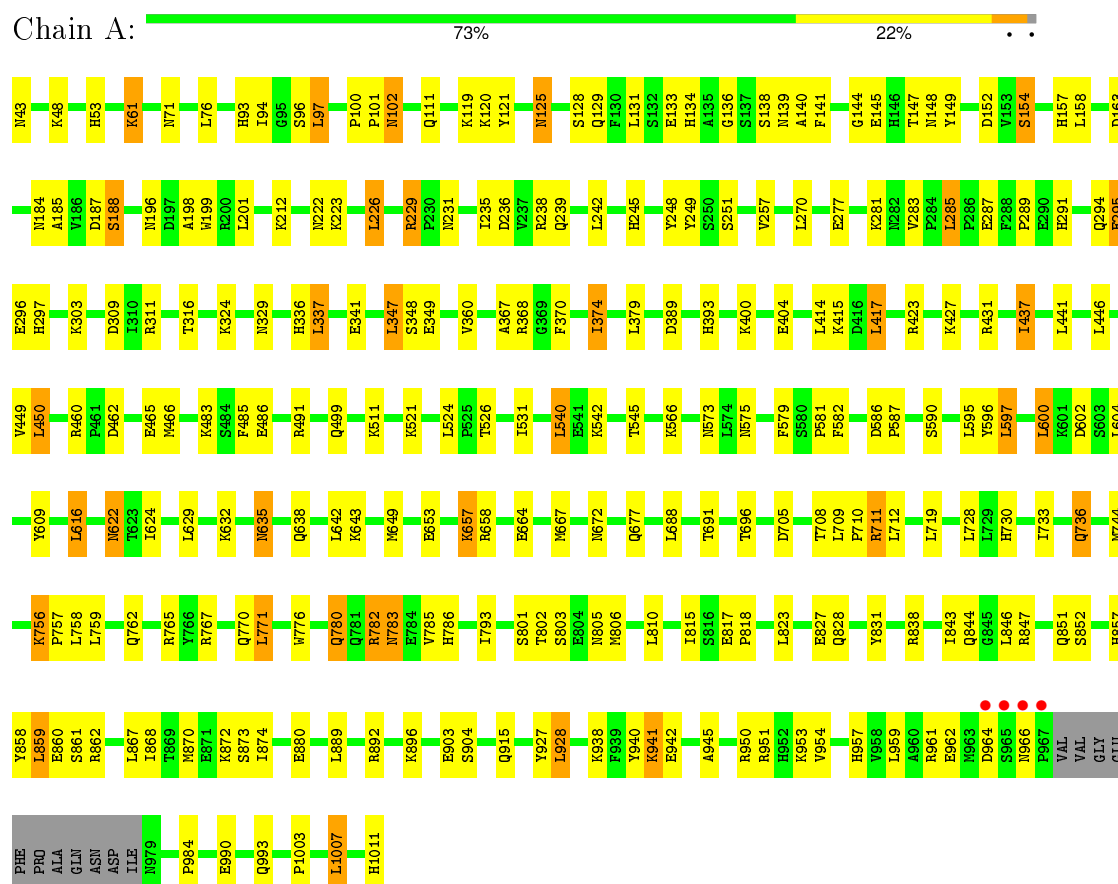
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	221	Total	O	0	0
			221	221		
4	D	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		

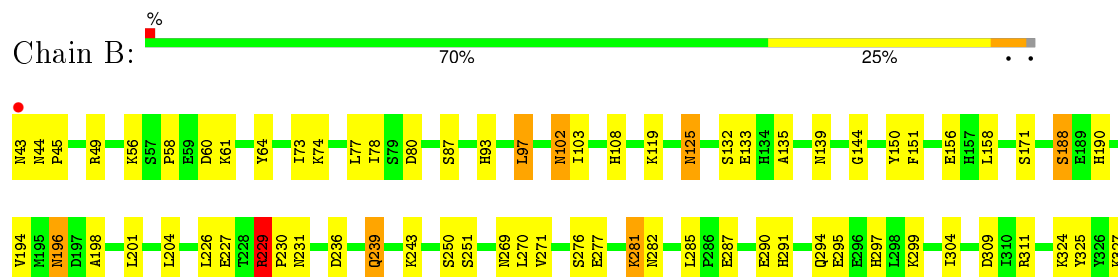
### 3 Residue-property plots

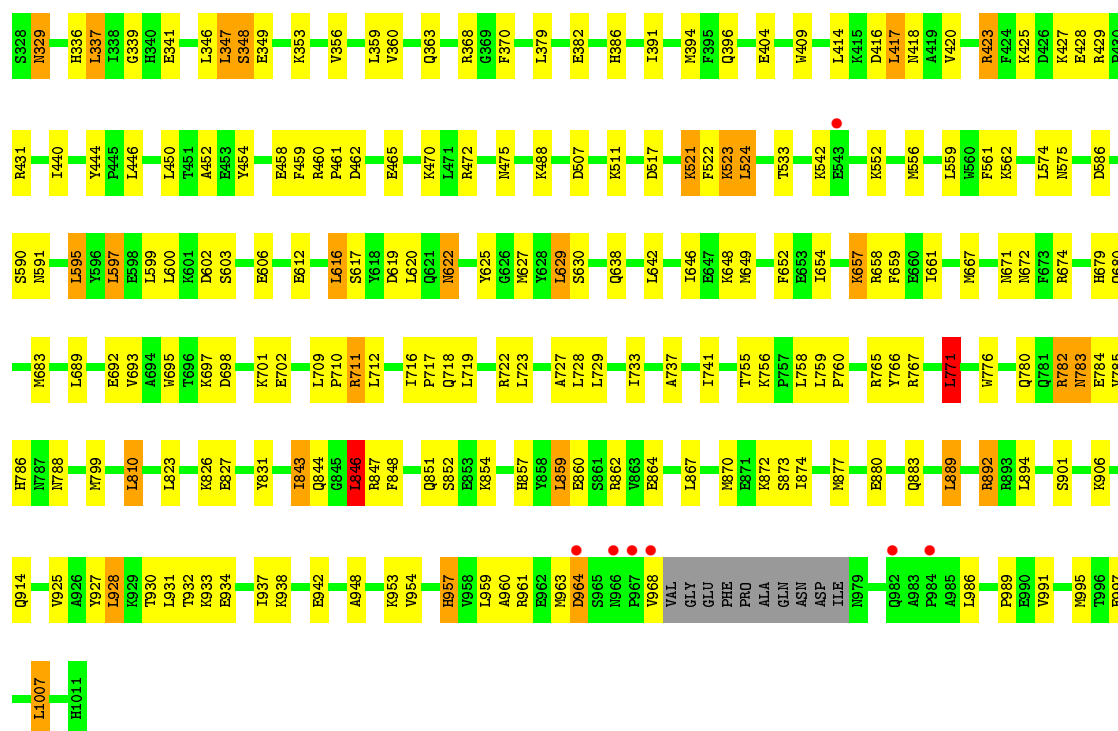
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

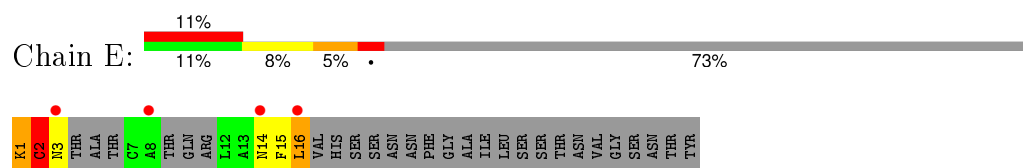




• Molecule 2: Islet amyloid polypeptide



• Molecule 2: Islet amyloid polypeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	262.87Å 262.87Å 90.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.69 – 2.91 49.68 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.69-2.91) 99.8 (49.68-2.91)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.224 0.183 , 0.224	Depositor DCC
$R_{free}$ test set	3956 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.4	EDS
Estimated twinning fraction	0.026 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 79012 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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 [i](#)

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

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	0.60	0/8033	0.71	3/10866 (0.0%)
1	B	0.57	0/8040	0.68	4/10876 (0.0%)
2	D	0.98	0/54	1.23	1/69 (1.4%)
2	E	1.05	0/69	1.11	1/88 (1.1%)
All	All	0.59	0/16196	0.70	9/21899 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	635	ASN	CB-CA-C	-8.45	93.50	110.40
1	B	964	ASP	CB-CA-C	6.74	123.89	110.40
1	A	226	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	285	LEU	CA-CB-CG	5.85	128.76	115.30
1	B	229	ARG	CG-CD-NE	5.13	122.56	111.80
2	E	2	CYS	CB-CA-C	-5.10	100.20	110.40
1	B	846	LEU	CA-CB-CG	5.06	126.94	115.30
2	D	1	LYS	CD-CE-NZ	-5.04	100.11	111.70
1	B	771	LEU	CA-CB-CG	5.00	126.81	115.30

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	7837	0	7773	156	0
1	B	7844	0	7782	206	0
2	D	55	0	61	10	0
2	E	71	0	70	9	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
4	A	123	0	0	30	0
4	B	221	0	0	58	0
4	D	2	0	0	3	0
4	E	1	0	0	3	0
All	All	16156	0	15686	371	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 12.

All (371) 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:892:ARG:HD3	4:A:2:HOH:O	1.41	1.14
1:A:296:GLU:HG3	4:A:1081:HOH:O	1.50	1.11
1:B:784:GLU:HG2	4:B:1054:HOH:O	1.49	1.09
2:D:15:PHE:O	4:D:432:HOH:O	1.67	1.09
2:E:15:PHE:O	4:E:334:HOH:O	1.69	1.08
1:A:868:ILE:HG13	4:A:1119:HOH:O	1.56	1.03
1:B:297:HIS:HE1	4:B:37:HOH:O	1.42	1.02
1:A:868:ILE:CG1	4:A:1119:HOH:O	2.07	0.99
1:B:523:LYS:CB	4:B:1203:HOH:O	2.09	0.99
1:B:353:LYS:HB2	4:B:1158:HOH:O	1.64	0.94
1:A:154:SER:HB3	4:A:1044:HOH:O	1.71	0.89
1:A:622:ASN:H	1:A:622:ASN:HD22	1.15	0.89
1:A:880:GLU:HA	4:A:1098:HOH:O	1.73	0.88
1:B:511:LYS:HB3	4:B:1164:HOH:O	1.73	0.87
1:B:523:LYS:HB2	4:B:1203:HOH:O	1.72	0.87
1:A:600:LEU:HD11	1:A:649:MET:HB3	1.57	0.85
1:A:102:ASN:HD22	1:A:102:ASN:H	1.24	0.84
1:B:733:ILE:HB	4:B:1176:HOH:O	1.74	0.84
1:B:843:ILE:HD12	1:B:843:ILE:N	1.94	0.83
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.40	0.82
4:B:1144:HOH:O	2:E:16:LEU:HB2	1.78	0.82
1:B:622:ASN:H	1:B:622:ASN:HD22	1.27	0.82
1:B:61:LYS:HA	1:B:61:LYS:HE2	1.61	0.81
1:B:281:LYS:HE3	4:B:1018:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:GLN:HA	4:B:1146:HOH:O	1.79	0.81
1:B:294:GLN:H	1:B:297:HIS:HD2	1.29	0.80
1:B:843:ILE:HG13	4:B:1183:HOH:O	1.83	0.79
1:B:231:ASN:HB3	4:B:1174:HOH:O	1.84	0.78
3:B:2:ZN:ZN	4:E:334:HOH:O	1.32	0.78
1:B:883:GLN:HB2	4:B:1127:HOH:O	1.84	0.78
3:A:1:ZN:ZN	4:D:432:HOH:O	1.32	0.78
1:A:622:ASN:H	1:A:622:ASN:ND2	1.82	0.77
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.20	0.77
1:A:770:GLN:HE21	1:A:1003:PRO:HB2	1.50	0.76
1:B:689:LEU:HD23	1:B:995:MET:HG3	1.67	0.75
1:A:499:GLN:HG3	4:A:1110:HOH:O	1.85	0.75
1:B:517:ASP:HB3	4:B:1213:HOH:O	1.86	0.74
1:B:87:SER:HB2	1:B:151:PHE:O	1.86	0.74
1:B:783:ASN:HD22	1:B:785:VAL:H	1.34	0.74
1:B:683:MET:SD	4:B:1146:HOH:O	2.46	0.74
1:B:602:ASP:OD1	1:B:658:ARG:HD3	1.85	0.73
1:A:892:ARG:CD	4:A:2:HOH:O	2.15	0.72
1:A:776:TRP:CD1	1:A:953:LYS:HG2	2.25	0.72
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.89	0.71
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.71	0.71
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.73	0.71
1:B:309:ASP:H	1:B:672:ASN:HD21	1.36	0.71
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.20	0.70
4:A:1022:HOH:O	2:D:15:PHE:HD2	1.73	0.70
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.55	0.70
1:A:868:ILE:HG12	4:A:1119:HOH:O	1.82	0.69
2:E:1:LYS:HG2	2:E:1:LYS:O	1.93	0.69
1:A:309:ASP:H	1:A:672:ASN:HD21	1.40	0.69
1:B:171:SER:HB2	4:B:1150:HOH:O	1.91	0.69
1:A:120:LYS:HE3	1:B:409:TRP:CD1	2.28	0.69
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.59	0.68
1:B:311:ARG:NH1	1:B:379:LEU:O	2.27	0.68
1:B:108:HIS:NE2	4:E:334:HOH:O	2.26	0.68
1:B:102:ASN:H	1:B:102:ASN:HD22	1.41	0.68
1:A:783:ASN:ND2	1:A:786:HIS:H	1.92	0.68
1:B:622:ASN:H	1:B:622:ASN:ND2	1.92	0.67
1:B:61:LYS:HE3	4:B:1188:HOH:O	1.93	0.67
1:B:119:LYS:HD3	4:B:1150:HOH:O	1.95	0.67
1:A:635:ASN:C	1:A:635:ASN:ND2	2.48	0.67
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:997:GLU:HG2	4:B:1104:HOH:O	1.94	0.66
1:A:283:VAL:HG12	4:A:1075:HOH:O	1.96	0.65
1:B:360:VAL:HA	2:E:1:LYS:HD3	1.77	0.65
1:A:196:ASN:ND2	1:A:199:TRP:H	1.95	0.65
1:A:941:LYS:HD2	4:A:1090:HOH:O	1.96	0.65
1:B:309:ASP:H	1:B:672:ASN:ND2	1.95	0.64
1:A:767:ARG:HG2	1:A:1007:LEU:HD13	1.79	0.64
2:D:1:LYS:HG3	2:D:1:LYS:O	1.97	0.64
1:B:517:ASP:CB	4:B:1213:HOH:O	2.43	0.64
1:A:667:MET:HE2	4:A:1032:HOH:O	1.95	0.64
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.80	0.64
1:A:309:ASP:H	1:A:672:ASN:ND2	1.95	0.63
1:B:960:ALA:HB3	1:B:963:MET:HB2	1.79	0.63
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.81	0.63
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.99	0.62
1:B:934:GLU:HG2	4:B:1071:HOH:O	2.00	0.62
1:B:783:ASN:ND2	1:B:785:VAL:H	1.98	0.61
1:B:61:LYS:HA	1:B:61:LYS:CE	2.29	0.60
1:A:196:ASN:HD22	1:A:199:TRP:H	1.47	0.60
1:B:646:ILE:HD13	1:B:649:MET:HE1	1.81	0.60
1:A:961:ARG:HD3	4:A:1102:HOH:O	2.01	0.60
1:B:997:GLU:CG	4:B:1104:HOH:O	2.49	0.60
1:A:756:LYS:HB2	1:A:757:PRO:CD	2.32	0.60
1:A:708:THR:OG1	1:A:711:ARG:HD3	2.02	0.60
1:A:294:GLN:H	1:A:297:HIS:HD2	1.48	0.60
1:B:423:ARG:CG	1:B:423:ARG:HH11	2.14	0.60
1:A:782:ARG:HD2	4:A:1033:HOH:O	2.01	0.59
1:A:667:MET:HG2	4:A:1043:HOH:O	2.01	0.59
1:A:134:HIS:HB3	4:A:1044:HOH:O	2.01	0.59
1:B:783:ASN:ND2	1:B:786:HIS:H	2.00	0.59
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.31	0.59
1:B:932:THR:OG1	1:B:934:GLU:HB2	2.02	0.58
1:B:892:ARG:CD	4:B:1072:HOH:O	2.50	0.58
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.83	0.58
1:B:843:ILE:N	1:B:843:ILE:CD1	2.63	0.58
1:B:229:ARG:NH1	4:B:1155:HOH:O	2.35	0.58
1:B:843:ILE:HG22	1:B:844:GLN:H	1.68	0.58
1:A:427:LYS:HE3	4:A:1096:HOH:O	2.02	0.58
1:B:45:PRO:HD2	4:B:1148:HOH:O	2.03	0.58
1:B:297:HIS:CE1	4:B:37:HOH:O	2.30	0.57
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.87	0.57
1:A:415:LYS:NZ	4:A:1086:HOH:O	2.37	0.57
1:A:303:LYS:HD3	1:A:485:PHE:CE2	2.40	0.57
1:B:667:MET:HG2	1:B:701:LYS:NZ	2.19	0.57
1:B:697:LYS:O	1:B:701:LYS:HB2	2.05	0.57
1:B:359:LEU:O	2:E:1:LYS:HE3	2.05	0.57
1:A:196:ASN:ND2	1:A:199:TRP:HD1	2.02	0.57
1:B:74:LYS:HG3	4:B:1034:HOH:O	2.05	0.57
1:B:667:MET:HG2	1:B:701:LYS:HZ3	1.70	0.56
1:A:880:GLU:HG3	1:B:327:LYS:HD2	1.87	0.56
1:B:250:SER:HB2	1:B:281:LYS:HB2	1.87	0.56
1:A:139:ASN:OD1	2:D:16:LEU:HB3	2.06	0.56
1:B:782:ARG:NH2	1:B:963:MET:O	2.39	0.56
1:B:767:ARG:HG2	1:B:1007:LEU:HD13	1.87	0.55
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.89	0.55
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.88	0.55
1:B:77:LEU:HD21	1:B:271:VAL:HG21	1.87	0.55
1:B:597:LEU:HG	1:B:620:LEU:HG	1.89	0.55
1:A:229:ARG:CG	1:A:229:ARG:HH11	2.13	0.55
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.90	0.54
1:B:446:LEU:HD12	1:B:446:LEU:H	1.72	0.54
1:B:991:VAL:HB	4:B:1014:HOH:O	2.08	0.54
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.41	0.54
1:A:97:LEU:HB2	1:A:144:GLY:O	2.07	0.54
1:A:102:ASN:ND2	1:A:102:ASN:H	2.01	0.54
1:B:648:LYS:O	1:B:652:PHE:HB2	2.08	0.54
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.89	0.54
1:A:129:GLN:O	1:A:133:GLU:HG2	2.07	0.54
1:B:843:ILE:HG22	1:B:844:GLN:N	2.23	0.53
1:A:616:LEU:HD21	1:A:638:GLN:HG3	1.88	0.53
1:A:245:HIS:O	1:A:249:TYR:HB2	2.09	0.53
1:A:336:HIS:CD2	1:A:337:LEU:HD13	2.40	0.53
1:A:860:GLU:OE2	1:A:957:HIS:HE1	1.92	0.53
1:B:711:ARG:NH2	4:B:1026:HOH:O	2.41	0.53
1:A:858:TYR:O	1:A:861:SER:HB3	2.09	0.53
1:B:646:ILE:HD13	1:B:649:MET:CE	2.38	0.52
1:B:521:LYS:HD2	4:B:35:HOH:O	2.08	0.52
1:B:386:HIS:HE1	4:B:1075:HOH:O	1.92	0.52
1:B:125:ASN:H	1:B:125:ASN:HD22	1.56	0.52
1:B:523:LYS:HB3	4:B:1203:HOH:O	1.94	0.52
1:A:843:ILE:HG22	1:A:844:GLN:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:HB2	1:A:757:PRO:HD2	1.91	0.52
1:A:349:GLU:OE2	1:A:521:LYS:HD3	2.10	0.52
1:A:184:ASN:HD21	1:A:223:LYS:HE2	1.74	0.52
4:A:1022:HOH:O	2:D:15:PHE:CD2	2.54	0.52
1:A:465:GLU:HG2	4:A:1052:HOH:O	2.10	0.52
1:B:139:ASN:OD1	2:E:16:LEU:HB3	2.10	0.52
1:A:196:ASN:HD21	1:A:198:ALA:HB3	1.75	0.52
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.45	0.52
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.92	0.52
1:A:102:ASN:HD22	1:A:102:ASN:N	1.96	0.51
1:B:654:ILE:CD1	1:B:654:ILE:N	2.73	0.51
1:A:730:HIS:HD2	1:A:904:SER:OG	1.92	0.51
1:A:857:HIS:HD2	4:A:1116:HOH:O	1.92	0.51
1:B:784:GLU:O	1:B:961:ARG:HG3	2.10	0.51
1:B:132:SER:HB3	4:B:1131:HOH:O	2.10	0.51
1:B:336:HIS:HD2	1:B:337:LEU:HD13	1.73	0.51
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.91	0.51
1:B:892:ARG:HD2	4:B:1072:HOH:O	2.10	0.51
1:B:892:ARG:HD3	4:B:1072:HOH:O	2.11	0.51
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.91	0.51
1:B:269:ASN:HB2	4:B:1041:HOH:O	2.09	0.51
1:A:341:GLU:OE1	2:D:1:LYS:NZ	2.44	0.51
1:B:657:LYS:O	1:B:661:ILE:HG12	2.10	0.51
1:B:277:GLU:HB3	4:B:1093:HOH:O	2.11	0.51
1:A:604:LEU:HA	4:A:1113:HOH:O	2.11	0.51
1:B:44:ASN:OD1	4:B:1148:HOH:O	2.19	0.50
1:B:243:LYS:HE3	4:B:1052:HOH:O	2.09	0.50
1:B:196:ASN:ND2	1:B:198:ALA:H	2.08	0.50
1:A:341:GLU:HG2	1:A:347:LEU:HD12	1.92	0.50
1:B:654:ILE:HD12	1:B:654:ILE:N	2.27	0.50
1:A:635:ASN:C	1:A:635:ASN:HD22	2.12	0.50
1:A:957:HIS:HD2	1:A:966:ASN:ND2	2.08	0.50
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.94	0.50
1:A:389:ASP:O	1:A:393:HIS:HD2	1.95	0.50
1:B:799:MET:HA	4:B:1183:HOH:O	2.10	0.50
1:A:677:GLN:NE2	1:A:851:GLN:HE22	2.10	0.50
1:A:119:LYS:HD2	4:A:1093:HOH:O	2.11	0.50
1:B:591:ASN:O	1:B:595:LEU:HD22	2.12	0.50
1:A:770:GLN:HE21	1:A:1003:PRO:CB	2.22	0.49
1:A:360:VAL:HA	2:D:1:LYS:HD3	1.93	0.49
1:A:801:SER:O	1:A:802:THR:C	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:TYR:CZ	1:B:765:ARG:HD2	2.47	0.49
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.46	0.49
1:B:968:VAL:HG11	1:B:989:PRO:HG3	1.93	0.49
1:A:635:ASN:O	1:A:635:ASN:ND2	2.44	0.49
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.48	0.49
1:B:49:ARG:HH12	1:B:446:LEU:HD13	1.78	0.49
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.95	0.49
1:A:184:ASN:ND2	1:A:223:LYS:HE2	2.27	0.49
1:A:951:ARG:HD3	4:A:1069:HOH:O	2.12	0.49
1:B:339:GLY:HA3	2:E:1:LYS:HD2	1.94	0.48
1:A:111:GLN:NE2	2:D:16:LEU:HB2	2.28	0.48
1:B:843:ILE:CG1	4:B:1183:HOH:O	2.51	0.48
1:B:646:ILE:HA	1:B:649:MET:HE3	1.94	0.48
1:B:44:ASN:OD1	1:B:45:PRO:HD2	2.13	0.48
1:A:961:ARG:HD2	1:A:962:GLU:OE1	2.13	0.48
1:A:815:ILE:HA	1:A:870:MET:HE2	1.94	0.48
1:B:425:LYS:HE2	1:B:428:GLU:OE2	2.13	0.48
1:B:49:ARG:HD2	4:B:1031:HOH:O	2.14	0.48
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.48	0.48
1:B:629:LEU:HD22	1:B:630:SER:N	2.29	0.48
1:B:58:PRO:HG2	4:B:1092:HOH:O	2.14	0.48
1:A:657:LYS:HB2	1:A:657:LYS:NZ	2.28	0.48
1:B:533:THR:HG23	4:B:18:HOH:O	2.13	0.48
1:A:581:PRO:HG2	1:A:582:PHE:CD1	2.49	0.47
1:A:579:PHE:HE2	1:A:765:ARG:HH22	1.62	0.47
1:B:324:LYS:HE3	1:B:325:TYR:CZ	2.49	0.47
1:A:843:ILE:HG22	1:A:844:GLN:N	2.28	0.47
1:B:196:ASN:C	1:B:196:ASN:HD22	2.18	0.47
1:B:97:LEU:HB2	1:B:144:GLY:O	2.14	0.47
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.61	0.47
1:B:295:GLU:OE1	1:B:295:GLU:HA	2.14	0.47
1:A:141:PHE:HA	2:D:14:ASN:O	2.15	0.47
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.63	0.47
1:B:61:LYS:HB2	4:B:1105:HOH:O	2.15	0.47
1:A:400:LYS:HE3	1:A:404:GLU:CG	2.45	0.47
1:B:239:GLN:OE1	1:B:243:LYS:HD2	2.15	0.46
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.96	0.46
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.50	0.46
1:B:843:ILE:H	1:B:843:ILE:CD1	2.28	0.46
1:B:423:ARG:CG	1:B:423:ARG:NH1	2.79	0.46
2:D:1:LYS:N	4:D:38:HOH:O	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:HIS:HB3	1:B:851:GLN:HB2	1.96	0.46
1:A:483:LYS:O	1:A:486:GLU:HG2	2.16	0.46
1:B:417:LEU:HD12	1:B:417:LEU:HA	1.79	0.46
1:B:329:ASN:HD21	1:B:363:GLN:HE22	1.61	0.46
1:B:683:MET:HE1	4:B:1185:HOH:O	2.15	0.46
1:A:289:PRO:HD2	4:A:41:HOH:O	2.14	0.46
1:B:671:ASN:O	1:B:674:ARG:HG2	2.16	0.46
1:B:561:PHE:HE1	1:B:733:ILE:HD12	1.80	0.46
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.32	0.46
1:B:889:LEU:HB3	1:B:928:LEU:HD11	1.98	0.46
1:B:810:LEU:HG	1:B:928:LEU:HD21	1.97	0.46
1:A:140:ALA:HA	1:A:148:ASN:O	2.16	0.46
1:A:711:ARG:HH21	1:A:711:ARG:CG	2.28	0.46
1:B:196:ASN:ND2	1:B:196:ASN:C	2.69	0.46
1:A:736:GLN:H	1:A:736:GLN:CD	2.19	0.46
1:A:61:LYS:HA	1:A:61:LYS:HD3	1.75	0.46
1:A:767:ARG:HG2	1:A:1007:LEU:CD1	2.45	0.46
1:A:417:LEU:HA	1:A:417:LEU:HD12	1.88	0.46
1:B:616:LEU:HD21	1:B:638:GLN:HG3	1.98	0.46
1:A:573:ASN:ND2	1:A:632:LYS:HG2	2.31	0.46
1:B:349:GLU:OE2	1:B:349:GLU:HA	2.16	0.46
1:B:446:LEU:HD12	1:B:446:LEU:N	2.30	0.45
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.97	0.45
1:A:597:LEU:HD12	1:A:597:LEU:HA	1.74	0.45
1:B:396:GLN:HG2	1:B:517:ASP:O	2.16	0.45
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.99	0.45
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.97	0.45
1:A:579:PHE:HE2	1:A:765:ARG:NH2	2.14	0.45
1:A:566:LYS:HD2	1:A:903:GLU:OE1	2.17	0.45
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.99	0.45
1:B:139:ASN:HB3	1:B:150:TYR:CE1	2.52	0.45
1:A:783:ASN:ND2	1:A:785:VAL:H	2.14	0.45
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.20	0.45
1:B:404:GLU:HG3	1:B:524:LEU:HD21	1.99	0.45
1:B:877:MET:O	1:B:933:LYS:HE2	2.16	0.45
1:A:121:TYR:OH	1:A:163:ASP:OD1	2.32	0.45
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.16	0.45
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.98	0.45
1:B:418:ASN:HB3	1:B:454:TYR:O	2.16	0.45
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.52	0.45
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.99	0.45
1:A:196:ASN:ND2	1:A:199:TRP:CD1	2.83	0.45
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.52	0.45
1:A:294:GLN:H	1:A:297:HIS:CD2	2.33	0.44
1:B:470:LYS:O	1:B:475:ASN:ND2	2.39	0.44
1:B:622:ASN:N	1:B:622:ASN:ND2	2.64	0.44
1:B:870:MET:O	1:B:874:ILE:HG13	2.17	0.44
1:A:780:GLN:HE22	1:A:959:LEU:HD11	1.82	0.44
1:A:145:GLU:OE2	1:A:367:ALA:HB1	2.17	0.44
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.52	0.44
1:A:316:THR:HG23	1:A:374:ILE:HG22	2.00	0.44
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.53	0.44
1:A:984:PRO:HD3	4:A:1119:HOH:O	2.18	0.44
1:B:760:PRO:HD2	4:B:1156:HOH:O	2.18	0.44
1:B:864:GLU:HG3	1:B:986:LEU:HD21	2.00	0.44
1:B:227:GLU:C	1:B:230:PRO:HD2	2.38	0.44
1:B:698:ASP:HA	1:B:701:LYS:HB3	2.00	0.44
1:B:416:ASP:O	1:B:420:VAL:HG23	2.18	0.44
1:B:488:LYS:HD2	4:B:1113:HOH:O	2.18	0.44
1:A:586:ASP:HB2	1:A:587:PRO:HD2	2.00	0.44
1:A:417:LEU:HD11	1:A:531:ILE:HD13	1.99	0.43
1:B:702:GLU:HB3	4:B:1205:HOH:O	2.17	0.43
1:B:612:GLU:HG3	1:B:617:SER:HB3	2.00	0.43
1:A:125:ASN:HD22	1:A:125:ASN:H	1.65	0.43
1:B:603:SER:OG	1:B:648:LYS:HE3	2.18	0.43
1:B:444:TYR:CE1	1:B:452:ALA:HB1	2.53	0.43
1:B:942:GLU:O	1:B:948:ALA:HB1	2.18	0.43
1:B:294:GLN:H	1:B:297:HIS:CD2	2.20	0.43
1:B:602:ASP:OD1	1:B:658:ARG:CD	2.62	0.43
1:B:860:GLU:OE2	1:B:957:HIS:HE1	2.01	0.43
1:B:575:ASN:O	1:B:727:ALA:HA	2.18	0.43
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.18	0.43
1:A:257:VAL:HG21	1:A:437:ILE:HB	2.01	0.43
1:B:523:LYS:CG	4:B:1203:HOH:O	2.55	0.43
1:B:507:ASP:O	1:B:511:LYS:HG3	2.18	0.43
1:A:806:MET:HE3	1:A:928:LEU:HG	2.01	0.43
1:B:784:GLU:CG	4:B:1054:HOH:O	2.33	0.42
1:B:93:HIS:HE1	1:B:368:ARG:NH2	2.17	0.42
1:A:231:ASN:HA	1:A:231:ASN:HD22	1.70	0.42
1:B:348:SER:OG	1:B:606:GLU:OE2	2.31	0.42
1:A:600:LEU:CD1	1:A:649:MET:HB3	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ARG:NH1	1:B:462:ASP:OD2	2.53	0.42
1:A:136:GLY:HA3	1:A:152:ASP:O	2.19	0.42
1:B:133:GLU:HG3	4:B:1131:HOH:O	2.20	0.42
1:B:425:LYS:HB3	1:B:425:LYS:NZ	2.35	0.42
1:B:204:LEU:CD2	1:B:304:ILE:HG12	2.50	0.42
1:A:71:ASN:HB2	1:A:251:SER:OG	2.19	0.42
1:B:959:LEU:HD13	1:B:964:ASP:O	2.19	0.42
1:A:157:HIS:CD2	4:A:1044:HOH:O	2.72	0.42
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.20	0.42
1:A:295:GLU:HA	1:A:295:GLU:OE1	2.20	0.42
1:B:857:HIS:HB2	1:B:968:VAL:HA	2.02	0.42
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.85	0.42
1:A:53:HIS:HE1	4:A:10:HOH:O	2.03	0.42
1:B:602:ASP:CG	1:B:658:ARG:HH11	2.23	0.42
1:B:933:LYS:O	1:B:937:ILE:HG12	2.20	0.42
1:A:915:GLN:O	1:A:1011:HIS:HB3	2.19	0.42
1:A:236:ASP:CG	1:A:239:GLN:HG2	2.40	0.42
1:B:723:LEU:HD12	1:B:755:THR:HG21	2.02	0.42
1:A:229:ARG:HG2	1:A:229:ARG:NH1	2.18	0.41
1:A:341:GLU:HB2	1:A:609:TYR:CG	2.55	0.41
1:A:374:ILE:HD13	1:A:374:ILE:O	2.19	0.41
1:B:722:ARG:NH2	1:B:756:LYS:HB2	2.35	0.41
1:B:767:ARG:HG2	1:B:1007:LEU:CD1	2.51	0.41
1:A:486:GLU:HB2	4:A:1055:HOH:O	2.19	0.41
1:A:803:SER:HA	1:A:927:TYR:CE2	2.55	0.41
1:B:236:ASP:OD1	1:B:236:ASP:C	2.58	0.41
1:B:429:ARG:HE	1:B:429:ARG:HB2	1.74	0.41
1:B:854:LYS:HB2	1:B:859:LEU:HD13	2.02	0.41
1:B:461:PRO:O	1:B:465:GLU:HG3	2.20	0.41
1:B:299:LYS:HE2	4:B:1025:HOH:O	2.20	0.41
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.49	0.41
1:B:64:TYR:CE2	1:B:78:ILE:HG12	2.55	0.41
1:B:843:ILE:H	1:B:843:ILE:HD12	1.75	0.41
2:E:2:CYS:O	2:E:3:ASN:C	2.59	0.41
1:B:391:ILE:O	1:B:394:MET:HB2	2.21	0.41
1:B:382:GLU:HB2	4:B:1035:HOH:O	2.19	0.41
1:B:597:LEU:HD21	1:B:627:MET:HG2	2.02	0.41
1:B:860:GLU:OE2	1:B:957:HIS:CE1	2.74	0.41
1:B:597:LEU:HD23	1:B:622:ASN:N	2.36	0.41
1:B:135:ALA:HA	1:B:892:ARG:CZ	2.50	0.41
1:A:870:MET:O	1:A:874:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ARG:HG2	4:B:1208:HOH:O	2.21	0.41
1:B:56:LYS:HD2	1:B:60:ASP:HB3	2.03	0.41
1:A:596:TYR:OH	1:A:649:MET:HB2	2.20	0.41
1:A:311:ARG:HD2	1:A:379:LEU:O	2.21	0.41
1:B:847:ARG:NH1	4:B:1110:HOH:O	2.46	0.41
1:A:238:ARG:NH1	1:A:242:LEU:HD11	2.35	0.41
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.50	0.40
1:A:860:GLU:OE2	1:A:957:HIS:CE1	2.74	0.40
1:B:711:ARG:HD3	4:B:1090:HOH:O	2.21	0.40
1:B:190:HIS:O	1:B:194:VAL:HG23	2.22	0.40
1:B:80:ASP:HA	4:B:1079:HOH:O	2.20	0.40
1:A:782:ARG:NH2	1:A:964:ASP:HA	2.36	0.40
1:A:100:PRO:HA	1:A:101:PRO:HD3	1.96	0.40
1:B:108:HIS:CD2	2:E:14:ASN:HB3	2.56	0.40
1:B:693:VAL:HB	1:B:766:TYR:CE2	2.57	0.40
1:B:737:ALA:O	1:B:741:ILE:HG13	2.22	0.40
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.84	0.40
1:A:793:ILE:O	1:A:847:ARG:HA	2.21	0.40
1:B:846:LEU:CD1	1:B:848:PHE:CE1	3.04	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	954/969 (98%)	908 (95%)	46 (5%)	0	100	100
1	B	955/969 (99%)	909 (95%)	46 (5%)	0	100	100
2	D	3/37 (8%)	3 (100%)	0	0	100	100
2	E	4/37 (11%)	4 (100%)	0	0	100	100
All	All	1916/2012 (95%)	1824 (95%)	92 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	854/863 (99%)	764 (90%)	90 (10%)	8	25
1	B	855/863 (99%)	774 (90%)	81 (10%)	11	30
2	D	6/31 (19%)	3 (50%)	3 (50%)	0	0
2	E	7/31 (23%)	4 (57%)	3 (43%)	0	0
All	All	1722/1788 (96%)	1545 (90%)	177 (10%)	9	26

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	48	LYS
1	A	61	LYS
1	A	76	LEU
1	A	96	SER
1	A	97	LEU
1	A	102	ASN
1	A	125	ASN
1	A	128	SER
1	A	154	SER
1	A	158	LEU
1	A	188	SER
1	A	201	LEU
1	A	212	LYS
1	A	226	LEU
1	A	229	ARG
1	A	235	ILE
1	A	270	LEU
1	A	277	GLU
1	A	281	LYS
1	A	285	LEU
1	A	287	GLU

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Mol	Chain	Res	Type
1	A	295	GLU
1	A	324	LYS
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	348	SER
1	A	374	ILE
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG
1	A	431	ARG
1	A	437	ILE
1	A	446	LEU
1	A	450	LEU
1	A	466	MET
1	A	491	ARG
1	A	511	LYS
1	A	524	LEU
1	A	526	THR
1	A	540	LEU
1	A	542	LYS
1	A	545	THR
1	A	575	ASN
1	A	590	SER
1	A	595	LEU
1	A	597	LEU
1	A	600	LEU
1	A	616	LEU
1	A	622	ASN
1	A	624	ILE
1	A	629	LEU
1	A	642	LEU
1	A	643	LYS
1	A	653	GLU
1	A	657	LYS
1	A	691	THR
1	A	705	ASP
1	A	711	ARG
1	A	712	LEU
1	A	719	LEU
1	A	728	LEU
1	A	733	ILE

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Mol	Chain	Res	Type
1	A	736	GLN
1	A	744	MET
1	A	756	LYS
1	A	758	LEU
1	A	771	LEU
1	A	780	GLN
1	A	782	ARG
1	A	783	ASN
1	A	810	LEU
1	A	823	LEU
1	A	838	ARG
1	A	846	LEU
1	A	859	LEU
1	A	867	LEU
1	A	872	LYS
1	A	873	SER
1	A	889	LEU
1	A	896	LYS
1	A	928	LEU
1	A	938	LYS
1	A	941	LYS
1	A	942	GLU
1	A	950	ARG
1	A	990	GLU
1	A	993	GLN
1	A	1007	LEU
1	B	43	ASN
1	B	97	LEU
1	B	102	ASN
1	B	103	ILE
1	B	125	ASN
1	B	156	GLU
1	B	158	LEU
1	B	188	SER
1	B	196	ASN
1	B	201	LEU
1	B	226	LEU
1	B	229	ARG
1	B	239	GLN
1	B	270	LEU
1	B	276	SER
1	B	281	LYS

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	285	LEU
1	B	287	GLU
1	B	290	GLU
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	348	SER
1	B	356	VAL
1	B	414	LEU
1	B	417	LEU
1	B	423	ARG
1	B	427	LYS
1	B	431	ARG
1	B	440	ILE
1	B	450	LEU
1	B	458	GLU
1	B	521	LYS
1	B	523	LYS
1	B	524	LEU
1	B	542	LYS
1	B	556	MET
1	B	562	LYS
1	B	590	SER
1	B	595	LEU
1	B	597	LEU
1	B	600	LEU
1	B	616	LEU
1	B	619	ASP
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	657	LYS
1	B	711	ARG
1	B	712	LEU
1	B	718	GLN
1	B	719	LEU
1	B	728	LEU
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	780	GLN

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Mol	Chain	Res	Type
1	B	782	ARG
1	B	783	ASN
1	B	788	ASN
1	B	810	LEU
1	B	823	LEU
1	B	826	LYS
1	B	843	ILE
1	B	846	LEU
1	B	859	LEU
1	B	867	LEU
1	B	872	LYS
1	B	873	SER
1	B	880	GLU
1	B	889	LEU
1	B	892	ARG
1	B	901	SER
1	B	906	LYS
1	B	914	GLN
1	B	928	LEU
1	B	930	THR
1	B	938	LYS
1	B	957	HIS
1	B	1007	LEU
2	D	1	LYS
2	D	2	CYS
2	D	12	LEU
2	E	1	LYS
2	E	2	CYS
2	E	16	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	102	ASN
1	A	111	GLN
1	A	125	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	294	GLN

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Mol	Chain	Res	Type
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	336	HIS
1	A	393	HIS
1	A	407	GLN
1	A	502	GLN
1	A	573	ASN
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	770	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	957	HIS
1	A	982	GLN
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	129	GLN
1	B	184	ASN
1	B	190	HIS
1	B	196	ASN
1	B	231	ASN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	329	ASN
1	B	336	HIS
1	B	363	GLN
1	B	386	HIS
1	B	393	HIS
1	B	407	GLN
1	B	502	GLN
1	B	573	ASN

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Mol	Chain	Res	Type
1	B	575	ASN
1	B	589	HIS
1	B	605	ASN
1	B	622	ASN
1	B	672	ASN
1	B	677	GLN
1	B	730	HIS
1	B	783	ASN
1	B	805	ASN
1	B	828	GLN
1	B	883	GLN
1	B	914	GLN
1	B	922	ASN
1	B	957	HIS
1	B	979	ASN
1	B	988	GLN
1	B	993	GLN
2	D	14	ASN

### 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

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	958/969 (98%)	-0.17	4 (0%) 93 92	38, 52, 68, 102	1 (0%)
1	B	959/969 (98%)	-0.09	8 (0%) 87 86	44, 57, 74, 103	1 (0%)
2	D	7/37 (18%)	1.67	1 (14%) 4 2	62, 103, 104, 104	0
2	E	10/37 (27%)	2.06	4 (40%) 0 0	84, 104, 105, 106	0
All	All	1934/2012 (96%)	-0.11	17 (0%) 85 84	38, 55, 73, 106	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	966	ASN	5.7
1	A	967	PRO	4.4
1	B	968	VAL	4.4
1	B	966	ASN	4.3
2	E	16	LEU	3.5
1	B	967	PRO	3.5
1	B	984	PRO	3.4
2	D	12	LEU	3.3
1	A	964	ASP	3.2
2	E	8	ALA	2.9
1	A	965	SER	2.7
1	B	964	ASP	2.6
1	B	43	ASN	2.4
2	E	3	ASN	2.4
1	B	543	GLU	2.3
1	B	982	GLN	2.2
2	E	14	ASN	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 [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
3	ZN	B	2	1/1	0.98	0.19	-0.56	2,2,2,2	0
3	ZN	A	1	1/1	0.96	0.17	-0.82	2,2,2,2	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.