



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:10 PM UTC

PDB ID : 3QZ2 / pdb_00003qz2
Title : The structure of cysteine-free human insulin degrading enzyme
Authors : Guo, Q.; Tang, W.J.
Deposited on : 2011-03-04
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

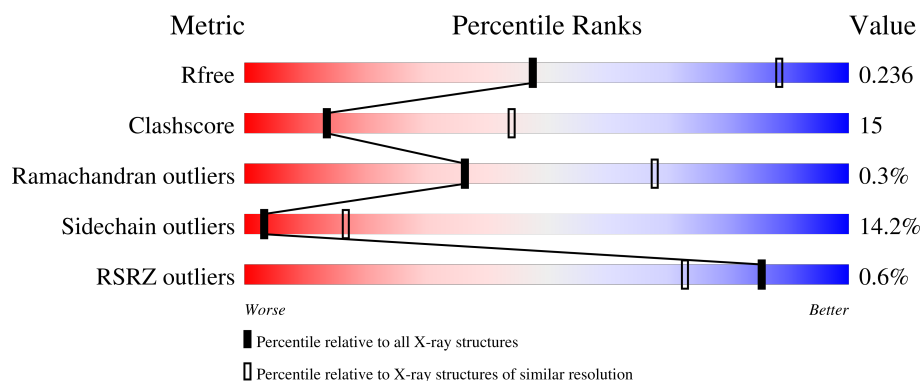
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	62% 29% 5% .
1	B	990	59% 30% 7% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15748 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	0
			7790	5019	1308	1441	22			
1	B	952	Total	C	N	O	S	0	0	0
			7780	5013	1305	1440	22			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	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
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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	94	Total O 94 94	0	0
3	B	82	Total O 82 82	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.07Å 262.07Å 90.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.20) 99.6 (50.00-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.172 , 0.241 0.173 , 0.236	Depositor DCC
R_{free} test set	2967 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15748	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.00	8/7984 (0.1%)	1.21	43/10800 (0.4%)
1	B	0.97	5/7972 (0.1%)	1.19	41/10782 (0.4%)
All	All	0.99	13/15956 (0.1%)	1.20	84/21582 (0.4%)

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	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	ILE	CG1-CD1	10.71	1.93	1.51
1	A	992	ILE	C-N	-8.68	1.22	1.33
1	A	545	THR	N-CA	6.12	1.50	1.45
1	B	707	VAL	CA-CB	5.69	1.59	1.53
1	A	545	THR	CA-C	5.50	1.57	1.52
1	A	764	VAL	CA-CB	5.35	1.60	1.54
1	A	750	ILE	CA-CB	5.28	1.60	1.54
1	A	577	GLU	CG-CD	5.25	1.65	1.52
1	A	640	ILE	CA-CB	5.20	1.60	1.54
1	A	146	HIS	CA-C	-5.12	1.46	1.52
1	B	764	VAL	CA-CB	5.07	1.61	1.54
1	B	1010	PRO	CA-C	5.07	1.59	1.52
1	B	305	VAL	CA-CB	5.05	1.59	1.53

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	626	GLY	N-CA-C	-12.10	95.94	112.52
1	A	993	GLN	N-CA-C	-10.51	98.96	112.93
1	B	626	GLY	N-CA-C	-10.38	97.93	111.52
1	A	992	ILE	O-C-N	-10.33	109.66	122.57
1	B	365	GLU	CB-CA-C	-9.45	93.50	109.65
1	A	1010	PRO	CB-CA-C	-8.96	97.49	110.75
1	A	99	ASP	CA-C-N	-8.78	113.25	119.66
1	A	99	ASP	C-N-CA	-8.78	113.25	119.66
1	A	293	PHE	N-CA-C	-8.08	93.78	107.99
1	A	171	SER	CA-C-N	-7.98	111.54	119.76
1	A	171	SER	C-N-CA	-7.98	111.54	119.76
1	A	856	PRO	CB-CA-C	-7.81	100.27	111.68
1	A	993	GLN	N-CA-CB	7.66	123.68	110.34
1	A	797	THR	CB-CA-C	-7.55	100.77	111.65
1	A	557	SER	N-CA-C	7.49	120.59	108.76
1	B	405	GLY	CA-C-N	7.44	129.14	119.84
1	B	405	GLY	C-N-CA	7.44	129.14	119.84
1	B	636	ASP	N-CA-C	7.30	119.93	111.02
1	B	534	ASN	N-CA-C	6.93	119.57	108.41
1	A	992	ILE	CA-C-N	6.72	134.22	122.79
1	A	992	ILE	C-N-CA	6.72	134.22	122.79
1	B	329	ASN	CA-C-N	-6.69	112.10	119.19
1	B	329	ASN	C-N-CA	-6.69	112.10	119.19
1	B	610	ALA	N-CA-C	-6.69	104.07	111.36
1	A	329	ASN	CA-C-N	6.69	126.19	119.24
1	A	329	ASN	C-N-CA	6.69	126.19	119.24
1	A	797	THR	N-CA-C	6.56	120.99	111.02
1	A	495	TRP	N-CA-C	6.38	119.22	111.82
1	A	854	LYS	CA-C-N	6.32	124.21	119.66
1	A	854	LYS	C-N-CA	6.32	124.21	119.66
1	A	636	ASP	N-CA-C	6.27	121.65	111.37
1	A	100	PRO	CA-C-N	-6.23	113.39	119.87
1	A	100	PRO	C-N-CA	-6.23	113.39	119.87
1	A	553	ASP	N-CA-C	6.20	117.88	110.44
1	B	873	SER	N-CA-C	6.06	117.89	111.28
1	B	519	ASN	CB-CA-C	6.05	118.81	110.34
1	A	1010	PRO	CA-C-N	6.04	132.57	121.70
1	A	1010	PRO	C-N-CA	6.04	132.57	121.70
1	A	249	TYR	N-CA-C	-6.01	97.99	110.80
1	A	691	THR	N-CA-C	-5.92	100.90	110.32
1	A	756	LYS	CA-C-N	5.86	125.79	119.76
1	A	756	LYS	C-N-CA	5.86	125.79	119.76
1	B	957	HIS	CA-C-N	-5.82	115.45	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	957	HIS	C-N-CA	-5.82	115.45	122.90
1	B	836	GLY	CA-C-N	5.79	125.74	119.78
1	B	836	GLY	C-N-CA	5.79	125.74	119.78
1	B	785	VAL	N-CA-C	5.72	116.92	112.12
1	A	75	VAL	CB-CA-C	-5.68	102.04	110.33
1	B	953	LYS	N-CA-C	5.56	117.49	108.26
1	B	545	THR	N-CA-C	5.55	117.67	110.40
1	A	116	LEU	N-CA-C	5.54	118.83	112.57
1	B	661	ILE	CB-CA-C	-5.53	104.58	112.22
1	B	444	TYR	CA-C-N	5.53	125.54	119.90
1	B	444	TYR	C-N-CA	5.53	125.54	119.90
1	B	459	PHE	CA-C-N	-5.47	116.07	123.46
1	B	459	PHE	C-N-CA	-5.47	116.07	123.46
1	A	410	VAL	CB-CA-C	-5.46	104.92	112.24
1	B	401	LEU	N-CA-C	-5.41	105.30	111.14
1	B	783	ASN	N-CA-C	-5.40	99.71	108.52
1	A	437	ILE	CB-CA-C	-5.39	105.07	111.97
1	A	197	ASP	N-CA-C	5.36	117.21	111.36
1	B	475	ASN	N-CA-C	5.33	116.83	110.44
1	B	243	LYS	N-CA-CB	5.32	117.87	109.94
1	B	780	GLN	N-CA-C	5.30	118.07	109.06
1	B	911	ILE	N-CA-C	5.21	115.42	110.53
1	A	962	GLU	N-CA-C	5.21	119.35	112.89
1	B	764	VAL	N-CA-C	5.21	116.78	108.87
1	B	547	TYR	CA-C-N	-5.20	114.44	119.90
1	B	547	TYR	C-N-CA	-5.20	114.44	119.90
1	A	604	LEU	N-CA-C	5.18	119.08	112.34
1	A	500	TYR	N-CA-C	5.14	116.10	108.60
1	A	691	THR	CA-C-N	5.12	127.45	120.54
1	A	691	THR	C-N-CA	5.12	127.45	120.54
1	A	368	ARG	N-CA-C	-5.11	102.34	109.96
1	B	452	ALA	CA-C-N	-5.11	112.19	122.55
1	B	452	ALA	C-N-CA	-5.11	112.19	122.55
1	B	464	ILE	N-CA-C	-5.09	104.82	110.62
1	B	453	GLU	CB-CA-C	5.08	119.72	110.72
1	A	448	GLU	N-CA-C	5.07	119.46	113.28
1	B	762	GLN	N-CA-C	-5.04	107.62	112.97
1	B	627	MET	N-CA-C	5.02	117.95	110.52
1	B	472	ARG	CA-C-N	5.00	126.10	119.84
1	B	472	ARG	C-N-CA	5.00	126.10	119.84
1	B	643	LYS	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	992	ILE	Peptide,Mainchain

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	7790	0	7725	216	0
1	B	7780	0	7717	241	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	94	0	0	38	0
3	B	82	0	0	20	0
All	All	15748	0	15442	454	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 15.

All (454) 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:50:ILE:CD1	1:B:50:ILE:CG1	1.93	1.44
1:B:782:ARG:HD2	3:B:1059:HOH:O	1.46	1.12
1:B:679:HIS:O	1:B:681:HIS:N	1.86	1.09
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.12	1.08
1:B:856:PRO:O	1:B:858:TYR:N	1.88	1.07
1:A:697:LYS:HE2	3:A:1048:HOH:O	1.56	1.04
1:A:855:PRO:HB2	1:A:857:HIS:CD2	1.92	1.04
1:B:53:HIS:CD2	3:B:1043:HOH:O	2.11	1.04
1:A:243:LYS:HG3	3:A:1075:HOH:O	1.57	1.03
1:A:879:GLU:HG3	3:A:1072:HOH:O	1.62	0.98
1:B:455:LEU:HD23	3:B:1046:HOH:O	1.67	0.93
1:B:624:ILE:HD13	1:B:624:ILE:H	1.31	0.93
1:A:623:THR:OG1	1:A:626:GLY:O	1.83	0.93
1:A:53:HIS:HE1	3:A:7:HOH:O	1.52	0.93
1:B:622:ASN:HD22	1:B:622:ASN:H	0.94	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:HIS:N	3:A:1090:HOH:O	2.04	0.91
1:B:298:LEU:HD13	1:B:475:ASN:HB2	1.52	0.90
1:B:196:ASN:C	1:B:196:ASN:HD22	1.81	0.88
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.55	0.88
1:B:164:ARG:HG3	1:B:164:ARG:HH11	1.38	0.87
1:B:446:LEU:HD22	1:B:446:LEU:H	1.39	0.87
1:B:601:LYS:HE2	1:B:620:LEU:O	1.72	0.87
1:B:623:THR:OG1	1:B:626:GLY:O	1.92	0.87
1:B:309:ASP:H	1:B:672:ASN:HD21	1.23	0.87
1:A:491:ARG:HG3	1:A:491:ARG:NH1	1.86	0.86
1:B:622:ASN:H	1:B:622:ASN:ND2	1.73	0.86
1:A:679:HIS:O	1:A:681:HIS:N	2.09	0.86
1:B:309:ASP:H	1:B:672:ASN:ND2	1.77	0.83
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.27	0.82
1:B:239:GLN:HB3	3:B:1034:HOH:O	1.79	0.81
1:B:50:ILE:CD1	1:B:50:ILE:CG2	2.59	0.81
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.62	0.80
1:B:783:ASN:ND2	1:B:786:HIS:H	1.80	0.78
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.31	0.77
1:A:622:ASN:HD22	1:A:622:ASN:H	1.32	0.77
1:A:537:ILE:HD11	3:A:3:HOH:O	1.84	0.77
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.66	0.76
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.18	0.76
1:A:674:ARG:HD2	3:A:1051:HOH:O	1.85	0.76
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.67	0.76
1:A:575:ASN:HB3	1:A:908:TRP:CZ3	2.21	0.76
1:A:814:ILE:HG21	1:A:874:ILE:HD11	1.66	0.76
1:B:294:GLN:H	1:B:297:HIS:HD2	1.33	0.76
1:A:309:ASP:H	1:A:672:ASN:HD21	1.34	0.75
1:A:466:MET:HE2	1:A:466:MET:O	1.87	0.75
1:A:656:GLU:OE2	1:A:709:LEU:HD23	1.86	0.74
1:B:624:ILE:H	1:B:624:ILE:CD1	2.00	0.74
1:A:637:LYS:HE3	3:A:1068:HOH:O	1.86	0.73
1:B:674:ARG:HD2	3:B:1040:HOH:O	1.89	0.73
1:B:365:GLU:HG2	3:B:1071:HOH:O	1.89	0.72
1:A:350:LEU:HB3	1:A:356:VAL:HG22	1.70	0.72
1:B:654:ILE:HD13	1:B:712:LEU:HD13	1.71	0.72
1:A:622:ASN:H	1:A:622:ASN:ND2	1.84	0.72
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.70	0.72
1:B:102:ASN:HD22	1:B:102:ASN:H	1.36	0.72
1:B:50:ILE:CD1	1:B:50:ILE:HG23	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.73	0.70
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.73	0.70
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.73	0.70
1:B:783:ASN:HD22	1:B:786:HIS:H	1.39	0.70
1:A:963:MET:HA	3:A:1097:HOH:O	1.90	0.70
1:B:950:ARG:HD2	3:B:1056:HOH:O	1.93	0.69
1:A:205:GLU:HB3	3:A:1091:HOH:O	1.93	0.69
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.93	0.69
1:B:43:ASN:HB2	3:B:21:HOH:O	1.92	0.69
1:B:622:ASN:HD22	1:B:622:ASN:N	1.76	0.69
1:B:268:THR:O	1:B:272:VAL:HG23	1.93	0.68
1:B:950:ARG:NE	3:B:1085:HOH:O	2.24	0.68
1:B:679:HIS:C	1:B:681:HIS:N	2.50	0.68
1:B:574:LEU:C	1:B:575:ASN:HD22	2.02	0.68
1:A:805:ASN:O	1:A:809:GLU:HG3	1.94	0.68
1:A:527:LYS:H	1:A:527:LYS:HD2	1.59	0.67
1:B:196:ASN:ND2	1:B:198:ALA:H	1.91	0.67
1:A:783:ASN:ND2	1:A:786:HIS:H	1.93	0.67
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.11	0.67
1:A:53:HIS:HD2	3:A:1022:HOH:O	1.76	0.66
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.76	0.66
1:B:86:SER:HB3	1:B:158:LEU:HG	1.76	0.66
1:B:943:MET:HG3	3:B:1090:HOH:O	1.96	0.66
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.78	0.65
1:A:187:ASP:OD1	1:A:222:ASN:HB2	1.97	0.65
1:B:100:PRO:HG2	1:B:103:ILE:HG13	1.77	0.65
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.95	0.65
1:B:737:ALA:O	1:B:741:ILE:HG12	1.96	0.65
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.32	0.65
1:B:578:PHE:CD2	1:B:725:ILE:HG12	2.32	0.64
1:B:50:ILE:CD1	1:B:50:ILE:CB	2.75	0.64
1:B:164:ARG:HH11	1:B:164:ARG:CG	2.08	0.64
1:B:654:ILE:HD11	1:B:716:ILE:HD11	1.80	0.64
1:A:205:GLU:HG3	1:A:293:PHE:HZ	1.63	0.64
1:B:866:PHE:O	1:B:869:THR:HB	1.98	0.64
1:B:196:ASN:C	1:B:196:ASN:ND2	2.51	0.63
1:A:415:LYS:HG3	1:A:456:LEU:HB2	1.79	0.63
1:B:93:HIS:HE1	1:B:368:ARG:NH2	1.96	0.63
1:A:196:ASN:C	1:A:196:ASN:ND2	2.55	0.63
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.33	0.63
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LYS:HD3	1:A:620:LEU:O	1.99	0.63
1:B:583:ALA:HB2	1:B:626:GLY:HA2	1.80	0.63
1:B:204:LEU:O	1:B:208:THR:HG23	1.99	0.62
1:B:179:LYS:HD2	1:B:237:VAL:HG12	1.80	0.62
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.82	0.62
1:A:294:GLN:O	1:A:298:LEU:HG	2.00	0.62
1:A:765:ARG:HD3	3:A:19:HOH:O	1.99	0.62
1:A:309:ASP:H	1:A:672:ASN:ND2	1.98	0.62
1:A:196:ASN:ND2	1:A:199:TRP:H	1.98	0.61
1:A:826:LYS:CE	3:A:1024:HOH:O	2.48	0.61
1:B:774:ARG:HB2	1:B:774:ARG:HH11	1.65	0.61
1:B:294:GLN:H	1:B:297:HIS:CD2	2.16	0.61
1:A:855:PRO:HB2	1:A:857:HIS:NE2	2.14	0.61
1:B:243:LYS:HE2	3:B:1034:HOH:O	2.00	0.61
1:B:575:ASN:HD22	1:B:575:ASN:N	1.98	0.61
1:A:892:ARG:CD	3:A:1076:HOH:O	2.48	0.61
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.31	0.61
1:A:691:THR:HG23	1:A:841:ASN:HD21	1.65	0.61
1:A:730:HIS:HD2	1:A:904:SER:OG	1.83	0.61
1:B:196:ASN:ND2	1:B:198:ALA:N	2.49	0.61
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.82	0.60
1:B:774:ARG:HB2	1:B:774:ARG:NH1	2.17	0.60
1:A:855:PRO:CB	1:A:857:HIS:NE2	2.65	0.60
1:B:333:TYR:CD2	1:B:464:ILE:HD12	2.38	0.59
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.36	0.59
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.37	0.59
1:B:847:ARG:NH1	3:B:1063:HOH:O	2.33	0.59
1:A:80:ASP:OD1	1:A:82:THR:HG23	2.03	0.59
1:A:295:GLU:HA	1:A:298:LEU:HD12	1.83	0.59
1:B:688:LEU:HD13	1:B:995:MET:HE1	1.85	0.59
1:A:102:ASN:H	1:A:102:ASN:HD22	1.51	0.58
1:A:691:THR:O	1:A:999:LYS:HE3	2.02	0.58
1:B:285:LEU:HD22	1:B:286:PRO:HD2	1.85	0.58
1:A:950:ARG:CD	3:A:13:HOH:O	2.52	0.58
1:A:814:ILE:HG21	1:A:874:ILE:CD1	2.33	0.57
1:A:84:ASP:OD2	1:A:896:LYS:HG3	2.03	0.57
1:A:892:ARG:HD3	3:A:1076:HOH:O	2.03	0.57
1:B:908:TRP:HA	1:B:908:TRP:CE3	2.39	0.57
1:A:238:ARG:NH1	1:A:242:LEU:HD11	2.20	0.57
1:B:665:ALA:HA	1:B:668:ARG:HH21	1.70	0.57
1:B:110:LEU:HD23	1:B:110:LEU:C	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:NH2	1:B:498:THR:HA	2.20	0.57
1:A:826:LYS:HE3	3:A:1024:HOH:O	2.04	0.57
1:A:805:ASN:HD22	1:A:844:GLN:NE2	2.00	0.56
1:A:843:ILE:HG12	1:A:1005:PHE:CD1	2.40	0.56
1:A:598:GLU:OE1	1:A:601:LYS:NZ	2.39	0.56
1:A:545:THR:HB	1:A:546:PRO:HD2	1.87	0.56
1:B:102:ASN:H	1:B:102:ASN:ND2	2.03	0.56
1:B:395:PHE:CE2	1:B:473:PRO:HD3	2.41	0.56
1:A:196:ASN:HD21	1:A:199:TRP:H	1.52	0.56
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.88	0.56
1:B:510:ILE:O	1:B:514:GLN:HG3	2.05	0.56
1:A:359:LEU:C	1:A:359:LEU:HD23	2.31	0.55
1:B:139:ASN:HB3	1:B:150:TYR:CE1	2.41	0.55
1:A:426:ASP:HB3	1:A:899:LYS:HB3	1.87	0.55
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.41	0.55
1:B:858:TYR:N	3:B:29:HOH:O	2.38	0.55
1:A:257:VAL:HG21	1:A:437:ILE:HB	1.87	0.55
1:A:674:ARG:CD	3:A:1051:HOH:O	2.51	0.55
1:A:950:ARG:HD2	3:A:13:HOH:O	2.05	0.55
1:B:196:ASN:HD21	1:B:198:ALA:H	1.55	0.55
1:A:879:GLU:CG	3:A:1072:HOH:O	2.35	0.55
1:A:179:LYS:HD2	1:A:237:VAL:HB	1.89	0.54
1:A:914:GLN:HA	1:A:916:TYR:CE1	2.42	0.54
1:A:96:SER:HB3	3:A:14:HOH:O	2.07	0.54
1:A:862:ARG:NH2	1:A:981:SER:O	2.40	0.54
1:B:164:ARG:HG3	1:B:164:ARG:NH1	2.18	0.54
1:B:309:ASP:N	1:B:672:ASN:HD21	2.01	0.54
1:A:491:ARG:HH11	1:A:491:ARG:CG	2.00	0.54
1:A:697:LYS:CE	3:A:1048:HOH:O	2.31	0.54
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.88	0.53
1:B:643:LYS:O	1:B:647:GLU:HB2	2.09	0.53
1:A:892:ARG:HD2	3:A:1076:HOH:O	2.09	0.53
1:A:466:MET:HE2	1:A:466:MET:C	2.34	0.53
1:A:559:LEU:HD22	1:A:742:MET:CB	2.39	0.53
1:A:776:TRP:NE1	1:A:953:LYS:HE2	2.24	0.53
1:A:230:PRO:HA	1:A:235:ILE:HD12	1.90	0.53
1:B:176:GLU:HG3	3:B:1075:HOH:O	2.07	0.53
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.43	0.53
1:A:591:ASN:O	1:A:595:LEU:HD23	2.08	0.53
1:A:855:PRO:CG	1:A:857:HIS:NE2	2.72	0.53
1:B:259:LEU:HD23	1:B:259:LEU:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.44	0.53
1:B:257:VAL:HG12	1:B:434:THR:HG22	1.89	0.53
1:B:881:ALA:O	1:B:884:LYS:HB2	2.08	0.53
1:A:294:GLN:H	1:A:297:HIS:HD2	1.55	0.53
1:B:188:SER:HB3	1:B:831:TYR:CB	2.39	0.53
1:B:743:GLN:HG3	1:B:747:ASP:OD1	2.08	0.53
1:A:407:GLN:HB3	1:A:409:TRP:CD1	2.44	0.53
1:B:490:ASP:OD1	1:B:491:ARG:HG3	2.09	0.53
1:B:164:ARG:CG	1:B:164:ARG:NH1	2.70	0.52
1:B:874:ILE:HA	1:B:877:MET:HG2	1.91	0.52
1:B:326:TYR:CD1	1:B:444:TYR:HE1	2.27	0.52
1:A:406:PRO:HD3	3:A:1095:HOH:O	2.09	0.52
1:A:582:PHE:CE2	1:A:718:GLN:HG3	2.45	0.52
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.56	0.52
1:B:934:GLU:O	1:B:938:LYS:HG3	2.09	0.52
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.40	0.52
1:A:784:GLU:O	1:A:961:ARG:HG3	2.10	0.51
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.92	0.51
1:B:654:ILE:HD11	1:B:716:ILE:CD1	2.40	0.51
1:B:329:ASN:HD21	1:B:363:GLN:HE22	1.58	0.51
1:A:164:ARG:HG3	1:A:164:ARG:HH11	1.75	0.51
1:B:50:ILE:HG23	1:B:50:ILE:HD13	1.93	0.51
1:B:791:ILE:O	1:B:791:ILE:HG23	2.10	0.51
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.44	0.51
1:A:855:PRO:CB	1:A:857:HIS:CD2	2.81	0.51
1:B:795:TYR:CE2	1:B:953:LYS:HD2	2.46	0.51
1:B:125:ASN:HD22	1:B:125:ASN:H	1.58	0.51
1:B:50:ILE:CG2	1:B:50:ILE:HD12	2.37	0.50
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.11	0.50
1:B:693:VAL:HG21	1:B:766:TYR:CE2	2.47	0.50
1:A:842:GLY:C	1:A:843:ILE:HD12	2.37	0.50
1:A:888:ALA:O	1:A:892:ARG:HG3	2.11	0.50
1:B:351:LYS:HE3	1:B:602:ASP:OD2	2.12	0.50
1:B:795:TYR:OH	1:B:864:GLU:OE2	2.29	0.50
1:A:316:THR:HB	1:A:374:ILE:HG22	1.92	0.50
1:A:465:GLU:CG	3:A:1095:HOH:O	2.59	0.50
1:A:827:GLU:CD	1:A:862:ARG:HH11	2.20	0.50
1:A:350:LEU:HB3	1:A:356:VAL:CG2	2.42	0.50
1:B:196:ASN:HD22	1:B:197:ASP:N	2.09	0.50
1:A:207:ALA:HB2	3:A:5:HOH:O	2.11	0.50
1:A:795:TYR:HE2	1:A:953:LYS:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:LYS:HE2	3:A:1024:HOH:O	2.12	0.50
1:B:298:LEU:HD13	1:B:475:ASN:CB	2.34	0.50
1:B:750:ILE:HD13	1:B:755:THR:O	2.12	0.49
1:B:908:TRP:HA	1:B:908:TRP:HE3	1.77	0.49
1:A:353:LYS:HD3	1:A:355:TRP:CZ3	2.47	0.49
1:B:803:SER:HB2	1:B:927:TYR:OH	2.11	0.49
1:A:1007:LEU:HD23	1:B:1000:ARG:HG2	1.94	0.49
1:B:80:ASP:O	1:B:261:ARG:HA	2.13	0.49
1:A:305:VAL:HB	1:A:499:GLN:HB2	1.95	0.49
3:A:1033:HOH:O	1:B:706:ASP:HB2	2.12	0.49
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.77	0.49
1:A:714:ALA:O	1:A:717:PRO:HD2	2.12	0.49
1:B:108:HIS:CE1	1:B:189:GLU:OE1	2.65	0.49
1:A:331:GLY:HA3	1:A:363:GLN:OE1	2.13	0.49
1:A:195:MET:HB2	1:A:786:HIS:CE1	2.48	0.49
1:A:559:LEU:HD11	1:A:729:LEU:HG	1.95	0.49
1:A:584:TYR:CZ	1:A:624:ILE:HG22	2.48	0.49
1:A:927:TYR:O	1:A:930:THR:HB	2.13	0.49
1:A:465:GLU:HG3	3:A:1095:HOH:O	2.13	0.48
1:A:476:VAL:HG22	1:A:477:ARG:N	2.27	0.48
1:B:102:ASN:C	1:B:103:ILE:HG12	2.38	0.48
1:A:806:MET:HE3	1:A:928:LEU:HG	1.95	0.48
1:B:100:PRO:CG	1:B:103:ILE:HG13	2.44	0.48
1:B:856:PRO:HA	1:B:859:LEU:HB2	1.95	0.48
1:A:303:LYS:HG2	1:A:485:PHE:CE2	2.49	0.48
1:A:777:PHE:N	1:A:777:PHE:CD1	2.82	0.48
1:A:788:ASN:O	1:A:960:ALA:HA	2.13	0.48
1:B:655:ASP:OD1	1:B:655:ASP:C	2.56	0.48
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.96	0.48
1:A:76:LEU:HB2	1:A:441:LEU:HD11	1.95	0.48
1:A:188:SER:HB3	1:A:831:TYR:CB	2.39	0.48
1:B:446:LEU:H	1:B:446:LEU:CD2	2.19	0.48
1:B:646:ILE:O	1:B:647:GLU:C	2.56	0.48
1:B:677:GLN:HE21	1:B:786:HIS:CE1	2.31	0.48
1:A:600:LEU:HD22	1:A:649:MET:HB2	1.96	0.48
1:A:689:LEU:HD21	1:A:995:MET:HG2	1.96	0.48
1:A:801:SER:O	1:A:802:THR:C	2.57	0.48
1:B:595:LEU:HD12	1:B:662:ILE:HG22	1.96	0.48
1:B:644:LYS:O	1:B:648:LYS:HB2	2.13	0.48
1:B:870:MET:O	1:B:874:ILE:HG12	2.14	0.48
1:A:534:ASN:OD1	1:A:534:ASN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ASP:OD1	1:A:706:ASP:N	2.47	0.47
1:B:108:HIS:O	1:B:111:GLU:HB3	2.14	0.47
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.97	0.47
1:A:923:THR:HG21	3:A:1040:HOH:O	2.14	0.47
1:B:135:ALA:HB2	1:B:888:ALA:HA	1.95	0.47
1:B:597:LEU:HD21	1:B:627:MET:HG2	1.95	0.47
1:A:53:HIS:CE1	3:A:7:HOH:O	2.40	0.47
1:B:77:LEU:HD21	1:B:271:VAL:HG21	1.95	0.47
1:A:298:LEU:HD13	1:A:475:ASN:CB	2.44	0.47
1:A:491:ARG:HD3	3:A:1053:HOH:O	2.14	0.47
1:B:97:LEU:HB2	1:B:144:GLY:O	2.14	0.47
1:A:855:PRO:HB2	1:A:857:HIS:HD2	1.69	0.47
1:A:586:ASP:HB2	1:B:762:GLN:NE2	2.30	0.47
1:A:462:ASP:O	1:A:466:MET:HB2	2.15	0.46
1:B:312:ASN:HB3	1:B:314:TYR:CE2	2.50	0.46
1:A:298:LEU:HD21	1:A:318:PRO:HG3	1.97	0.46
1:B:295:GLU:OE2	1:B:295:GLU:HA	2.14	0.46
1:A:508:GLU:HA	1:A:511:LYS:HB2	1.97	0.46
1:A:591:ASN:O	1:A:595:LEU:CD2	2.62	0.46
1:A:795:TYR:CE2	1:A:953:LYS:HD2	2.50	0.46
1:B:76:LEU:HB3	1:B:257:VAL:HG22	1.97	0.46
1:B:667:MET:SD	1:B:701:LYS:HG3	2.55	0.46
1:A:345:SER:OG	1:A:348:SER:HB2	2.16	0.46
1:B:810:LEU:HG	1:B:928:LEU:HD21	1.97	0.46
1:B:347:LEU:HD13	3:B:18:HOH:O	2.15	0.46
1:B:930:THR:O	1:B:930:THR:HG22	2.15	0.46
1:A:272:VAL:O	1:A:273:LYS:C	2.59	0.46
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.97	0.46
1:A:597:LEU:HD12	1:A:597:LEU:HA	1.54	0.46
1:A:776:TRP:CE2	1:A:953:LYS:HE2	2.51	0.46
1:B:417:LEU:HD11	1:B:531:ILE:HD12	1.98	0.46
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.50	0.46
1:A:125:ASN:H	1:A:125:ASN:HD22	1.63	0.46
1:B:196:ASN:HD21	1:B:198:ALA:HB3	1.80	0.46
1:B:852:SER:CB	1:B:859:LEU:HD21	2.46	0.46
1:A:92:VAL:HG22	1:A:254:MET:HG2	1.97	0.45
1:B:311:ARG:NH2	1:B:664:GLU:OE1	2.43	0.45
1:B:359:LEU:C	1:B:359:LEU:HD23	2.41	0.45
1:A:592:MET:O	1:A:593:ALA:C	2.60	0.45
1:A:792:GLU:HA	1:A:848:PHE:O	2.16	0.45
1:A:870:MET:O	1:A:874:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:O	1:B:668:ARG:HD2	2.16	0.45
1:B:693:VAL:CG2	1:B:766:TYR:CE2	3.00	0.45
1:B:801:SER:O	1:B:805:ASN:CG	2.59	0.45
1:A:329:ASN:N	1:A:330:PRO:CD	2.79	0.45
1:A:446:LEU:O	1:A:449:VAL:HG22	2.15	0.45
1:B:912:ILE:C	1:B:914:GLN:H	2.23	0.45
1:B:200:ARG:HH21	1:B:498:THR:HA	1.81	0.45
1:A:759:LEU:HD11	1:B:702:GLU:HG2	1.97	0.45
1:B:674:ARG:CD	3:B:1040:HOH:O	2.55	0.45
1:A:94:ILE:CG2	1:A:95:GLY:N	2.78	0.45
1:A:433:TYR:O	1:A:437:ILE:HG12	2.17	0.45
1:A:793:ILE:HG21	1:A:795:TYR:CZ	2.52	0.45
1:B:53:HIS:HD2	3:B:1043:HOH:O	1.73	0.45
1:A:250:SER:HB2	1:A:281:LYS:HB2	1.98	0.45
1:A:291:HIS:ND1	1:A:292:PRO:HD2	2.32	0.45
1:B:673:PHE:C	1:B:675:ALA:H	2.25	0.45
1:A:840:ALA:O	1:A:841:ASN:C	2.59	0.44
3:A:1033:HOH:O	1:B:706:ASP:CB	2.65	0.44
1:B:413:GLU:OE2	1:B:527:LYS:HD2	2.17	0.44
1:B:889:LEU:HB3	1:B:928:LEU:HD11	1.99	0.44
1:B:229:ARG:HA	1:B:229:ARG:HD3	1.90	0.44
1:B:313:LEU:HD11	1:B:391:ILE:HD11	1.99	0.44
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.51	0.44
1:A:415:LYS:HA	1:A:456:LEU:HD12	1.98	0.44
1:A:609:TYR:CE2	1:A:613:LEU:HD11	2.52	0.44
1:B:665:ALA:HA	1:B:668:ARG:NH2	2.33	0.44
1:B:933:LYS:O	1:B:937:ILE:HG12	2.18	0.44
1:A:505:ILE:O	1:A:506:PRO:C	2.61	0.44
1:A:584:TYR:CE2	1:A:624:ILE:HG22	2.53	0.44
1:A:756:LYS:HB2	1:A:757:PRO:HD2	1.99	0.44
1:B:50:ILE:HD12	1:B:50:ILE:HG21	2.00	0.44
1:B:685:TYR:CZ	1:B:781:GLN:HG3	2.52	0.44
1:A:121:TYR:OH	1:A:163:ASP:OD1	2.25	0.44
1:B:782:ARG:NH1	1:B:961:ARG:O	2.51	0.44
1:A:99:ASP:O	1:A:217:LYS:NZ	2.49	0.43
1:A:597:LEU:O	1:A:601:LYS:HG3	2.18	0.43
1:A:715:PHE:CZ	1:A:719:LEU:HD22	2.53	0.43
1:B:162:LEU:HD23	1:B:270:LEU:HD11	2.00	0.43
1:B:688:LEU:HD23	1:B:694:ALA:HB1	2.00	0.43
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.66	0.43
1:A:43:ASN:C	1:A:43:ASN:ND2	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ARG:O	1:A:691:THR:OG1	2.36	0.43
1:A:74:LYS:NZ	3:A:28:HOH:O	2.50	0.43
1:A:782:ARG:HG2	1:A:959:LEU:HD12	2.00	0.43
1:A:961:ARG:HD2	1:A:962:GLU:OE1	2.18	0.43
1:A:275:PHE:O	1:A:278:VAL:HG23	2.18	0.43
1:A:351:LYS:HE3	1:A:602:ASP:OD2	2.18	0.43
1:B:73:ILE:HG12	1:B:254:MET:HB2	2.00	0.43
1:B:747:ASP:O	1:B:751:GLU:HB2	2.18	0.43
1:B:782:ARG:HH12	1:B:961:ARG:HA	1.84	0.43
1:B:798:ASP:HB3	1:B:804:GLU:HG2	2.00	0.43
1:B:849:ILE:O	1:B:850:ILE:HG13	2.18	0.43
1:B:586:ASP:O	1:B:587:PRO:C	2.62	0.43
1:B:686:LEU:HD12	1:B:686:LEU:HA	1.84	0.43
1:B:311:ARG:HB3	1:B:379:LEU:HB2	2.01	0.43
1:B:943:MET:CG	3:B:1090:HOH:O	2.63	0.43
1:A:574:LEU:HD22	1:A:729:LEU:HD22	2.00	0.43
1:A:756:LYS:HE2	1:A:756:LYS:HB3	1.76	0.43
1:A:893:ARG:HD2	1:A:893:ARG:HA	1.78	0.43
1:A:596:TYR:OH	1:A:649:MET:O	2.37	0.43
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.43	0.43
1:B:776:TRP:NE1	1:B:953:LYS:HE2	2.34	0.43
1:A:248:TYR:O	1:A:250:SER:N	2.52	0.42
1:A:950:ARG:HD3	3:A:13:HOH:O	2.15	0.42
1:B:367:ALA:HB3	1:B:370:PHE:CE2	2.54	0.42
1:A:299:LYS:HG2	1:A:510:ILE:HD11	2.01	0.42
1:B:122:PRO:O	1:B:123:LYS:C	2.60	0.42
1:B:960:ALA:HB3	1:B:963:MET:HG3	2.00	0.42
1:B:298:LEU:HD21	1:B:318:PRO:HG3	2.01	0.42
1:A:53:HIS:CD2	3:A:1022:HOH:O	2.59	0.42
1:B:674:ARG:NE	3:B:1040:HOH:O	2.50	0.42
1:B:855:PRO:O	1:B:858:TYR:HB3	2.20	0.42
1:A:602:ASP:OD2	1:A:658:ARG:NH1	2.53	0.42
1:B:591:ASN:O	1:B:595:LEU:HD22	2.19	0.42
1:A:329:ASN:N	1:A:330:PRO:HD2	2.35	0.42
1:A:415:LYS:HE2	1:A:415:LYS:HB3	1.86	0.42
1:B:74:LYS:O	1:B:255:ALA:HA	2.20	0.42
1:B:162:LEU:HD23	1:B:270:LEU:CD1	2.49	0.42
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.54	0.42
1:B:392:LEU:O	1:B:396:GLN:HG3	2.20	0.42
1:B:673:PHE:CD1	1:B:676:GLU:HG3	2.55	0.42
1:B:767:ARG:HG3	1:B:1007:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:HG11	1:A:377:VAL:HG11	2.02	0.42
1:B:852:SER:HB2	1:B:859:LEU:HD21	2.02	0.42
1:B:948:ALA:HB3	1:B:951:ARG:HB2	2.02	0.42
1:A:205:GLU:HG3	1:A:293:PHE:CZ	2.50	0.42
1:B:341:GLU:HG2	1:B:347:LEU:CD1	2.48	0.42
1:B:701:LYS:HE3	1:B:701:LYS:HB3	1.82	0.42
1:A:160:GLY:O	1:A:164:ARG:HG3	2.19	0.42
1:A:616:LEU:HD21	1:A:638:GLN:HG3	2.01	0.42
1:A:635:ASN:C	1:A:635:ASN:ND2	2.78	0.42
1:A:646:ILE:O	1:A:647:GLU:C	2.61	0.42
1:A:622:ASN:HD22	1:A:622:ASN:N	2.10	0.42
1:A:843:ILE:HG12	1:A:1005:PHE:CG	2.55	0.42
1:A:864:GLU:HG3	1:A:986:LEU:HD11	2.01	0.42
1:B:409:TRP:CE2	1:B:410:VAL:HG23	2.55	0.42
1:A:298:LEU:O	1:A:300:GLN:HG2	2.20	0.41
1:A:612:GLU:HA	1:A:616:LEU:O	2.20	0.41
1:B:815:ILE:HG22	1:B:870:MET:HE2	2.02	0.41
1:B:907:TYR:O	1:B:908:TRP:C	2.63	0.41
1:A:151:PHE:CD1	1:A:151:PHE:C	2.97	0.41
1:B:597:LEU:HD12	1:B:597:LEU:HA	1.92	0.41
1:B:867:LEU:HD12	1:B:867:LEU:HA	1.90	0.41
1:B:86:SER:CB	1:B:158:LEU:HG	2.48	0.41
1:B:289:PRO:HD2	1:B:290:GLU:H	1.85	0.41
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.89	0.41
1:B:65:ARG:HB3	1:B:264:LEU:HD22	2.02	0.41
1:B:425:LYS:NZ	1:B:425:LYS:HB3	2.35	0.41
1:B:760:PRO:O	1:B:763:LEU:HB2	2.21	0.41
1:A:139:ASN:HB3	1:A:150:TYR:OH	2.21	0.41
1:A:690:MET:O	1:A:768:GLU:HA	2.20	0.41
1:A:756:LYS:HB2	1:A:757:PRO:CD	2.50	0.41
1:B:329:ASN:C	1:B:329:ASN:HD22	2.29	0.41
1:B:838:ARG:HG3	1:B:847:ARG:HD3	2.03	0.41
1:A:997:GLU:HG2	1:A:1000:ARG:NH1	2.36	0.41
1:B:49:ARG:HG2	1:B:49:ARG:NH1	2.36	0.41
1:B:800:GLN:HB3	1:B:805:ASN:HD21	1.86	0.41
1:A:527:LYS:HD2	1:A:527:LYS:N	2.33	0.41
1:A:555:ALA:HB1	1:A:757:PRO:HB3	2.03	0.41
1:A:600:LEU:CD2	1:A:649:MET:HB2	2.50	0.41
1:B:53:HIS:CG	1:B:54:ILE:N	2.89	0.41
1:B:223:LYS:HB2	1:B:223:LYS:HE3	1.86	0.41
1:B:1009:LYS:HA	1:B:1010:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LYS:HE2	3:A:1086:HOH:O	2.20	0.41
1:A:171:SER:O	1:A:172:PRO:C	2.59	0.41
1:A:459:PHE:CE2	1:A:461:PRO:HG3	2.55	0.41
1:B:327:LYS:HG3	3:B:1032:HOH:O	2.21	0.41
1:B:691:THR:HG23	1:B:841:ASN:HD21	1.85	0.41
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.86	0.41
1:A:463:LEU:HD23	1:A:463:LEU:HA	1.90	0.40
1:B:77:LEU:CD2	1:B:271:VAL:HG21	2.51	0.40
1:B:466:MET:O	1:B:466:MET:HG2	2.20	0.40
1:B:627:MET:HE3	1:B:627:MET:HB2	1.92	0.40
1:B:671:ASN:O	1:B:674:ARG:HG2	2.20	0.40
1:A:119:LYS:HB2	1:A:171:SER:HB3	2.04	0.40
1:A:350:LEU:CB	1:A:356:VAL:HG22	2.47	0.40
1:B:196:ASN:HD22	1:B:198:ALA:N	2.19	0.40
1:B:565:ASP:OD2	1:B:566:LYS:HG3	2.21	0.40
1:B:624:ILE:HD13	1:B:624:ILE:N	2.15	0.40
1:B:767:ARG:CG	1:B:1007:LEU:HD13	2.52	0.40
1:B:575:ASN:N	1:B:575:ASN:ND2	2.67	0.40
1:B:912:ILE:C	1:B:914:GLN:N	2.79	0.40
1:A:569:LEU:HD12	3:A:1030:HOH:O	2.20	0.40
1:B:114:LEU:HD12	1:B:149:TYR:CZ	2.56	0.40
1:B:448:GLU:O	1:B:452:ALA:HB2	2.21	0.40
1:A:200:ARG:NH2	1:A:498:THR:HA	2.36	0.40
1:B:123:LYS:HB3	1:B:126:GLU:HB2	2.02	0.40
1:B:155:HIS:CE1	1:B:156:GLU:HG2	2.56	0.40
1:B:199:TRP:O	1:B:200:ARG:C	2.63	0.40
1:B:311:ARG:HA	1:B:481:VAL:O	2.22	0.40
1:B:640:ILE:H	1:B:640:ILE:HG12	1.69	0.40
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.57	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	947/990 (96%)	881 (93%)	65 (7%)	1 (0%)	48	79
1	B	944/990 (95%)	876 (93%)	63 (7%)	5 (0%)	24	59
All	All	1891/1980 (96%)	1757 (93%)	128 (7%)	6 (0%)	36	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	946	VAL
1	A	228	THR
1	B	406	PRO
1	B	405	GLY
1	B	587	PRO
1	B	791	ILE

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	847/879 (96%)	742 (88%)	105 (12%)	4	21
1	B	846/879 (96%)	711 (84%)	135 (16%)	2	13
All	All	1693/1758 (96%)	1453 (86%)	240 (14%)	3	17

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	50	ILE
1	A	57	SER
1	A	74	LYS
1	A	76	LEU
1	A	82	THR
1	A	97	LEU
1	A	102	ASN
1	A	111	GLU
1	A	116	LEU

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Mol	Chain	Res	Type
1	A	123	LYS
1	A	125	ASN
1	A	145	GLU
1	A	158	LEU
1	A	159	GLU
1	A	177	SER
1	A	188	SER
1	A	194	VAL
1	A	196	ASN
1	A	201	LEU
1	A	212	LYS
1	A	226	LEU
1	A	243	LYS
1	A	250	SER
1	A	252	ASN
1	A	270	LEU
1	A	277	GLU
1	A	285	LEU
1	A	287	GLU
1	A	316	THR
1	A	324	LYS
1	A	337	LEU
1	A	352	SER
1	A	388	GLU
1	A	392	LEU
1	A	408	GLU
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	420	VAL
1	A	429	ARG
1	A	449	VAL
1	A	450	LEU
1	A	460	ARG
1	A	466	MET
1	A	486	GLU
1	A	491	ARG
1	A	501	LYS
1	A	507	ASP
1	A	510	ILE
1	A	511	LYS
1	A	512	LYS

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Mol	Chain	Res	Type
1	A	515	ASN
1	A	518	LEU
1	A	519	ASN
1	A	534	ASN
1	A	558	LYS
1	A	582	PHE
1	A	588	LEU
1	A	595	LEU
1	A	597	LEU
1	A	616	LEU
1	A	622	ASN
1	A	625	TYR
1	A	629	LEU
1	A	642	LEU
1	A	648	LYS
1	A	649	MET
1	A	657	LYS
1	A	658	ARG
1	A	677	GLN
1	A	683	MET
1	A	691	THR
1	A	697	LYS
1	A	705	ASP
1	A	711	ARG
1	A	712	LEU
1	A	718	GLN
1	A	728	LEU
1	A	735	LYS
1	A	744	MET
1	A	756	LYS
1	A	764	VAL
1	A	771	LEU
1	A	782	ARG
1	A	783	ASN
1	A	793	ILE
1	A	801	SER
1	A	810	LEU
1	A	817	GLU
1	A	838	ARG
1	A	846	LEU
1	A	853	GLU
1	A	859	LEU

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Mol	Chain	Res	Type
1	A	862	ARG
1	A	867	LEU
1	A	873	SER
1	A	889	LEU
1	A	899	LYS
1	A	901	SER
1	A	914	GLN
1	A	923	THR
1	A	928	LEU
1	A	959	LEU
1	A	1007	LEU
1	B	43	ASN
1	B	48	LYS
1	B	50	ILE
1	B	52	ASN
1	B	61	LYS
1	B	67	LEU
1	B	76	LEU
1	B	92	VAL
1	B	94	ILE
1	B	96	SER
1	B	97	LEU
1	B	102	ASN
1	B	103	ILE
1	B	111	GLU
1	B	124	GLU
1	B	125	ASN
1	B	158	LEU
1	B	164	ARG
1	B	177	SER
1	B	188	SER
1	B	196	ASN
1	B	201	LEU
1	B	212	LYS
1	B	226	LEU
1	B	229	ARG
1	B	237	VAL
1	B	243	LYS
1	B	256	VAL
1	B	270	LEU
1	B	282	ASN
1	B	285	LEU

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Mol	Chain	Res	Type
1	B	316	THR
1	B	327	LYS
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	356	VAL
1	B	360	VAL
1	B	374	ILE
1	B	412	GLN
1	B	414	LEU
1	B	417	LEU
1	B	425	LYS
1	B	427	LYS
1	B	431	ARG
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	457	GLU
1	B	458	GLU
1	B	460	ARG
1	B	465	GLU
1	B	466	MET
1	B	470	LYS
1	B	472	ARG
1	B	473	PRO
1	B	502	GLN
1	B	510	ILE
1	B	511	LYS
1	B	512	LYS
1	B	517	ASP
1	B	523	LYS
1	B	524	LEU
1	B	534	ASN
1	B	540	LEU
1	B	575	ASN
1	B	587	PRO
1	B	595	LEU
1	B	597	LEU
1	B	602	ASP
1	B	603	SER
1	B	616	LEU
1	B	622	ASN

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Mol	Chain	Res	Type
1	B	624	ILE
1	B	629	LEU
1	B	635	ASN
1	B	637	LYS
1	B	640	ILE
1	B	642	LEU
1	B	643	LYS
1	B	644	LYS
1	B	648	LYS
1	B	649	MET
1	B	653	GLU
1	B	657	LYS
1	B	663	LYS
1	B	668	ARG
1	B	669	SER
1	B	674	ARG
1	B	677	GLN
1	B	681	HIS
1	B	691	THR
1	B	693	VAL
1	B	712	LEU
1	B	728	LEU
1	B	733	ILE
1	B	744	MET
1	B	751	GLU
1	B	759	LEU
1	B	765	ARG
1	B	768	GLU
1	B	770	GLN
1	B	771	LEU
1	B	774	ARG
1	B	788	ASN
1	B	791	ILE
1	B	799	MET
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	846	LEU
1	B	859	LEU
1	B	861	SER
1	B	873	SER
1	B	874	ILE

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Mol	Chain	Res	Type
1	B	875	GLU
1	B	889	LEU
1	B	898	LYS
1	B	900	LEU
1	B	901	SER
1	B	906	LYS
1	B	908	TRP
1	B	912	ILE
1	B	923	THR
1	B	924	GLU
1	B	928	LEU
1	B	929	LYS
1	B	934	GLU
1	B	942	GLU
1	B	954	VAL
1	B	962	GLU
1	B	980	LEU
1	B	993	GLN
1	B	996	THR
1	B	1007	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	239	GLN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	336	HIS
1	A	376	ASN
1	A	399	GLN
1	A	412	GLN
1	A	442	HIS

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Mol	Chain	Res	Type
1	A	502	GLN
1	A	514	GLN
1	A	575	ASN
1	A	622	ASN
1	A	672	ASN
1	A	718	GLN
1	A	730	HIS
1	A	762	GLN
1	A	783	ASN
1	A	786	HIS
1	A	805	ASN
1	A	813	GLN
1	A	821	ASN
1	A	828	GLN
1	A	841	ASN
1	A	885	HIS
1	A	988	GLN
1	B	52	ASN
1	B	53	HIS
1	B	93	HIS
1	B	125	ASN
1	B	134	HIS
1	B	148	ASN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	252	ASN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	312	ASN
1	B	329	ASN
1	B	386	HIS
1	B	407	GLN
1	B	412	GLN
1	B	475	ASN
1	B	502	GLN
1	B	515	ASN
1	B	534	ASN
1	B	575	ASN
1	B	591	ASN
1	B	605	ASN

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Mol	Chain	Res	Type
1	B	622	ASN
1	B	672	ASN
1	B	677	GLN
1	B	718	GLN
1	B	730	HIS
1	B	743	GLN
1	B	752	HIS
1	B	762	GLN
1	B	770	GLN
1	B	783	ASN
1	B	786	HIS
1	B	805	ASN
1	B	828	GLN
1	B	841	ASN
1	B	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 oligosaccharides 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	953/990 (96%)	-0.54	6 (0%) 85 73	11, 25, 40, 60	0
1	B	952/990 (96%)	-0.50	6 (0%) 85 73	14, 27, 41, 61	0
All	All	1905/1980 (96%)	-0.52	12 (0%) 85 73	11, 26, 41, 61	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	857	HIS	4.7
1	A	295	GLU	3.9
1	B	52	ASN	3.8
1	B	53	HIS	3.6
1	A	43	ASN	2.8
1	A	764	VAL	2.4
1	B	626	GLY	2.4
1	A	296	GLU	2.3
1	B	43	ASN	2.3
1	B	764	VAL	2.1
1	B	365	GLU	2.1
1	A	542	LYS	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	1	1/1	0.99	0.03	27,27,27,27	0
2	ZN	B	2	1/1	0.99	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.