Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 08:50 PM EST

PDB ID	:	3N57
Title	:	Crystal Structure of human Insulin-degrading enzyme (IDE) in complex with human atrial natriuretic peptide (ANP)
Authors	:	Funke, T.; Guo, Q.; Tang, W.-J.
Deposited on	:	2010-05-24
Resolution	:	3.03 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:

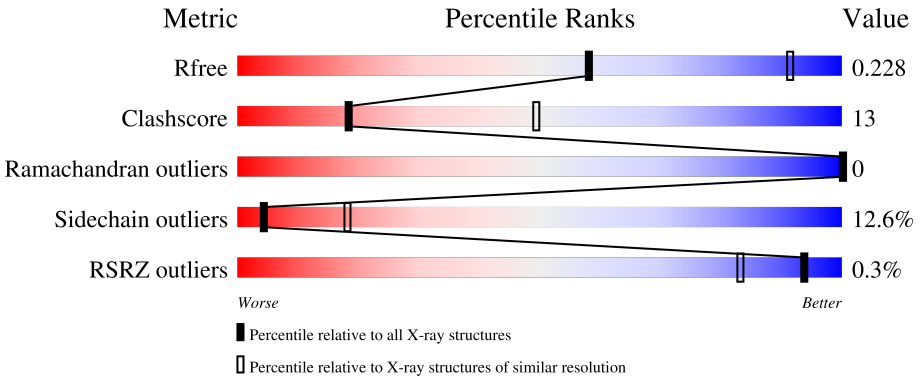
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 <=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	67% 24% 5% .
1	B	990	68% 23% 5% .
2	C	28	. 7% 89%
2	D	28	. 7% 89%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15718 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	954	Total	C	N	O	S	0	0	0
			7803	5026	1311	1444	22			
1	B	953	Total	C	N	O	S	0	0	0
			7799	5025	1310	1442	22			

There are 52 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	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

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

- Molecule 2 is a protein called Atrial natriuretic factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			25	15	6	4			
2	D	3	Total	C	N	O	0	0	0
			25	15	6	4			

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

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

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

- Molecule 4 is water.

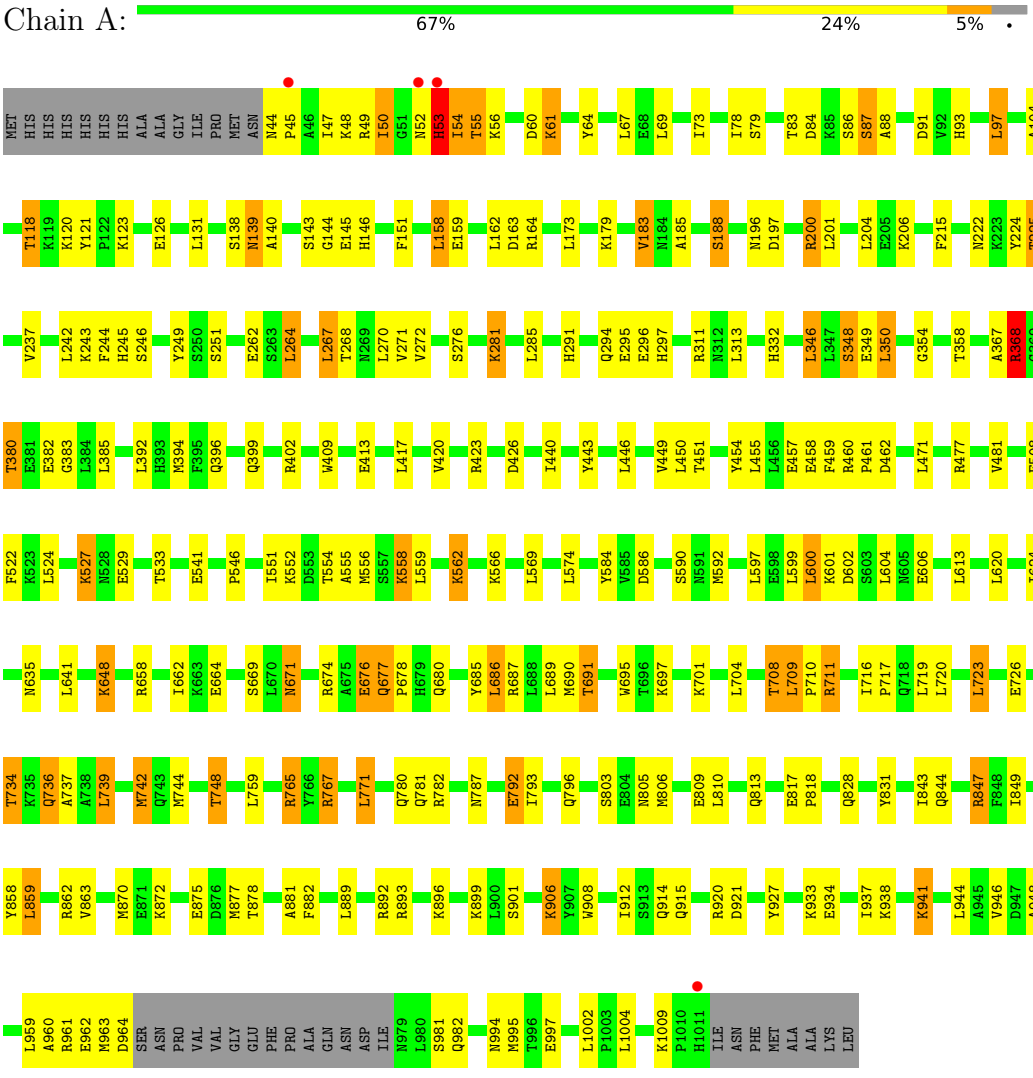
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	B	38	Total O 38 38	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

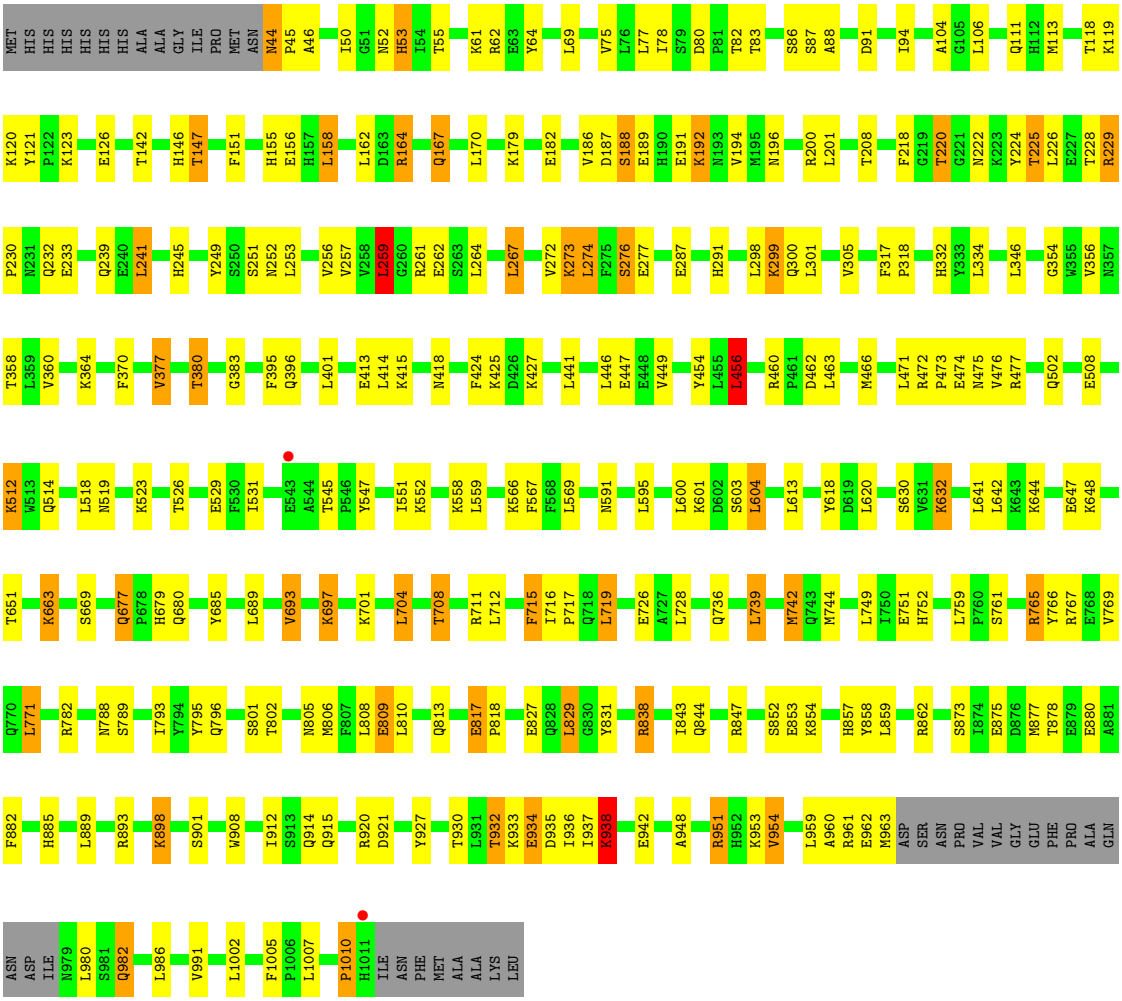
• Molecule 1: Insulin-degrading enzyme

Chain A:



• Molecule 1: Insulin-degrading enzyme

Chain B:



• Molecule 2: Atrial natriuretic factor

Chain C: 7% 89%

• Molecule 2: Atrial natriuretic factor

Chain D: 7% 89%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	264.10Å 264.10Å 91.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.96 – 3.03 29.96 – 3.03	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.96-3.03) 92.7 (29.96-3.03)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	5.71 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.242 0.194 , 0.228	Depositor DCC
R_{free} test set	1542 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 24.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15718	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.44	0/7996	0.67	9/10815 (0.1%)
1	B	0.52	5/7994 (0.1%)	0.74	12/10813 (0.1%)
2	C	0.67	0/24	1.38	1/30 (3.3%)
2	D	0.58	0/24	1.14	0/30
All	All	0.48	5/16038 (0.0%)	0.71	22/21688 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	938	LYS	CD-CE	13.96	1.86	1.51
1	B	938	LYS	CE-NZ	13.18	1.82	1.49
1	B	761	SER	CB-OG	6.59	1.50	1.42
1	B	632	LYS	CE-NZ	5.67	1.63	1.49
1	B	1010	PRO	C-N	-5.56	1.21	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	53	HIS	CB-CA-C	18.53	147.46	110.40
1	B	1010	PRO	O-C-N	-16.82	95.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	53	HIS	N-CA-C	-15.97	67.89	111.00
1	A	53	HIS	N-CA-C	-15.61	68.84	111.00
1	A	53	HIS	CB-CA-C	15.22	140.85	110.40
1	B	52	ASN	N-CA-C	15.00	151.50	111.00
1	B	1010	PRO	CA-C-N	12.32	144.30	117.20
1	B	52	ASN	CB-CA-C	-11.49	87.42	110.40
1	A	54	ILE	N-CA-C	-9.31	85.87	111.00
1	B	53	HIS	N-CA-CB	9.12	127.01	110.60
1	A	53	HIS	C-N-CA	8.70	143.46	121.70
1	B	53	HIS	C-N-CA	8.67	143.38	121.70
1	B	50	ILE	CB-CA-C	-8.28	95.03	111.60
1	A	627	MET	CB-CA-C	-7.39	95.62	110.40
1	A	54	ILE	CB-CA-C	6.68	124.96	111.60
1	B	259	LEU	CA-CB-CG	6.64	130.57	115.30
1	B	1010	PRO	C-N-CA	6.05	136.83	121.70
1	A	110	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	723	LEU	CA-CB-CG	5.65	128.31	115.30
2	C	2	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	456	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	368	ARG	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	HIS	Peptide
1	B	1010	PRO	Peptide
1	B	53	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7803	0	7745	208	0
1	B	7799	0	7742	209	0
2	C	25	0	31	3	0
2	D	25	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	0	2	0
4	B	38	0	0	3	0
All	All	15718	0	15549	415	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 13.

All (415) 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:938:LYS:CE	1:B:938:LYS:CD	1.86	1.50
1:A:938:LYS:HA	1:A:941:LYS:NZ	1.51	1.22
1:B:934:GLU:O	1:B:938:LYS:CD	1.88	1.16
1:A:625:TYR:OH	1:A:765:ARG:HG3	1.54	1.07
1:B:960:ALA:H	1:B:963:MET:HE3	1.16	1.04
1:B:142:THR:HG22	1:B:147:THR:HB	1.39	1.02
1:B:380:THR:HG22	1:B:383:GLY:H	1.22	1.01
1:A:938:LYS:CA	1:A:941:LYS:HZ2	1.76	0.99
1:B:317:PHE:CE1	1:B:476:VAL:HG22	1.98	0.97
1:A:938:LYS:HA	1:A:941:LYS:HZ2	1.02	0.96
1:B:938:LYS:CD	1:B:938:LYS:H	1.79	0.95
1:A:118:THR:HG22	1:A:121:TYR:H	1.31	0.94
1:B:601:LYS:HE2	1:B:620:LEU:O	1.70	0.91
1:A:915:GLN:HE21	1:A:920:ARG:HH22	1.22	0.87
1:A:915:GLN:NE2	1:A:920:ARG:HH22	1.73	0.86
1:B:765:ARG:CG	1:B:765:ARG:HH11	1.87	0.86
1:A:938:LYS:CA	1:A:941:LYS:NZ	2.33	0.85
1:A:744:MET:O	1:A:748:THR:HG22	1.76	0.85
1:A:687:ARG:O	1:A:691:THR:HG22	1.75	0.85
1:A:55:THR:HG22	1:A:451:THR:CG2	2.08	0.84
1:B:472:ARG:O	1:B:476:VAL:HG23	1.77	0.84
1:B:938:LYS:H	1:B:938:LYS:HD3	1.41	0.84
1:A:708:THR:HG23	1:A:710:PRO:HD2	1.59	0.84
1:B:796:GLN:NE2	1:B:1005:PHE:CE2	2.46	0.83
1:A:55:THR:CG2	1:A:451:THR:HG21	2.07	0.83
1:A:597:LEU:HD11	1:A:627:MET:HG2	1.59	0.83
1:A:53:HIS:O	1:A:54:ILE:HD13	1.80	0.81
1:B:91:ASP:OD2	1:B:146:HIS:HD2	1.64	0.81
1:B:196:ASN:O	1:B:200:ARG:HG3	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLN:HE21	1:B:502:GLN:HE21	1.29	0.80
1:B:829:LEU:O	1:B:852:SER:HB2	1.80	0.80
1:B:938:LYS:CD	1:B:938:LYS:N	2.45	0.80
1:B:715:PHE:CE1	1:B:719:LEU:HG	2.16	0.80
1:B:118:THR:HG21	1:B:167:GLN:HB3	1.64	0.79
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.62	0.79
1:B:960:ALA:N	1:B:963:MET:HE3	1.96	0.79
1:A:206:LYS:HD3	1:A:215:PHE:O	1.83	0.79
1:B:298:LEU:HD13	1:B:475:ASN:HA	1.65	0.78
1:A:937:ILE:O	1:A:941:LYS:HD3	1.82	0.78
2:D:3:ARG:HG2	2:D:3:ARG:HH11	1.49	0.77
1:B:94:ILE:O	1:B:147:THR:HG22	1.84	0.77
1:A:708:THR:CG2	1:A:711:ARG:HD3	2.15	0.77
1:B:208:THR:CG2	1:B:477:ARG:HH22	1.98	0.77
1:B:796:GLN:NE2	1:B:1005:PHE:HE2	1.80	0.77
1:B:113:MET:HE3	1:B:182:GLU:HB3	1.66	0.76
1:B:272:VAL:O	1:B:276:SER:HB2	1.86	0.76
1:A:52:ASN:O	1:A:53:HIS:HB2	1.85	0.76
1:A:625:TYR:CZ	1:A:765:ARG:CD	2.69	0.76
1:A:780:GLN:HE21	1:A:959:LEU:HD11	1.50	0.76
1:B:932:THR:HG22	1:B:935:ASP:H	1.51	0.75
1:A:91:ASP:OD2	1:A:146:HIS:HD2	1.67	0.75
1:B:354:GLY:O	1:B:380:THR:HG21	1.86	0.75
1:B:938:LYS:N	1:B:938:LYS:HD2	2.01	0.74
1:B:113:MET:CE	1:B:182:GLU:HB3	2.17	0.74
1:A:451:THR:HB	1:A:455:LEU:HD12	1.70	0.73
1:A:601:LYS:HE2	1:A:620:LEU:O	1.88	0.73
1:B:938:LYS:H	1:B:938:LYS:HD2	1.53	0.73
1:A:711:ARG:HG2	1:A:711:ARG:HH11	1.54	0.73
1:A:625:TYR:HH	1:A:765:ARG:HG3	1.49	0.73
1:B:765:ARG:HH11	1:B:765:ARG:HG2	1.54	0.72
1:B:142:THR:HG22	1:B:147:THR:CB	2.19	0.72
1:B:224:TYR:CE2	1:B:229:ARG:HD2	2.25	0.71
1:B:87:SER:HB2	1:B:151:PHE:O	1.90	0.71
1:A:787:ASN:HD21	1:A:962:GLU:HB2	1.55	0.71
1:B:782:ARG:NH1	1:B:961:ARG:O	2.23	0.71
1:B:960:ALA:H	1:B:963:MET:CE	1.98	0.71
1:A:708:THR:HG22	1:A:711:ARG:H	1.55	0.71
1:A:457:GLU:OE1	1:B:878:THR:OG1	2.06	0.70
1:B:208:THR:HG22	1:B:477:ARG:HH22	1.56	0.70
1:A:625:TYR:CE1	1:A:765:ARG:HD3	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASP:HB3	1:A:899:LYS:HG2	1.73	0.69
1:B:396:GLN:HE22	1:B:519:ASN:HD22	1.39	0.69
1:A:55:THR:HG21	1:A:451:THR:HG21	1.73	0.69
1:A:602:ASP:OD2	1:A:658:ARG:HD3	1.93	0.69
1:A:938:LYS:HA	1:A:941:LYS:HZ1	1.51	0.68
1:A:592:MET:HE1	1:A:711:ARG:HB3	1.75	0.68
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.74	0.68
1:A:938:LYS:O	1:A:941:LYS:NZ	2.26	0.68
1:B:104:ALA:O	1:B:225:THR:CG2	2.42	0.68
1:B:118:THR:HG21	1:B:167:GLN:CG	2.24	0.67
1:A:792:GLU:HG2	1:A:849:ILE:HG12	1.76	0.67
1:B:715:PHE:CD1	1:B:715:PHE:C	2.66	0.67
1:A:53:HIS:O	1:A:54:ILE:CD1	2.42	0.67
1:A:262:GLU:HB2	1:A:267:LEU:HD13	1.76	0.66
1:A:771:LEU:H	1:A:796:GLN:HE22	1.43	0.66
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.76	0.66
1:B:300:GLN:NE2	1:B:502:GLN:HE21	1.94	0.66
1:B:118:THR:HG21	1:B:167:GLN:CB	2.26	0.66
1:B:927:TYR:O	1:B:930:THR:HB	1.96	0.66
1:A:734:THR:HG23	1:A:736:GLN:HG2	1.77	0.65
1:A:813:GLN:HE22	1:A:892:ARG:NH2	1.94	0.65
1:B:915:GLN:HE21	1:B:920:ARG:HH22	1.43	0.65
1:A:79:SER:HB2	1:A:264:LEU:HD13	1.77	0.65
1:A:734:THR:CG2	1:A:736:GLN:HG2	2.26	0.65
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.97	0.65
1:A:159:GLU:HG3	1:A:270:LEU:HD11	1.77	0.65
1:A:104:ALA:O	1:A:225:THR:CG2	2.44	0.65
1:B:796:GLN:HE22	1:B:1005:PHE:HE2	1.43	0.65
1:A:55:THR:HG22	1:A:451:THR:HG23	1.78	0.65
1:B:715:PHE:CZ	1:B:719:LEU:HG	2.31	0.65
1:A:146:HIS:HE1	1:A:443:TYR:OH	1.80	0.65
1:B:708:THR:HG22	1:B:711:ARG:HB2	1.80	0.64
1:A:592:MET:CE	1:A:711:ARG:HB3	2.26	0.64
1:B:474:GLU:O	1:B:475:ASN:CB	2.46	0.64
1:B:441:LEU:HD13	1:B:449:VAL:HG11	1.80	0.64
1:A:711:ARG:HH11	1:A:711:ARG:CG	2.11	0.63
1:B:472:ARG:O	1:B:476:VAL:CG2	2.44	0.63
1:A:164:ARG:HG3	1:A:164:ARG:HH11	1.63	0.63
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.80	0.62
1:B:44:ASN:ND2	1:B:46:ALA:H	1.97	0.62
1:B:708:THR:HG22	1:B:711:ARG:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:THR:HG22	1:B:226:LEU:HG	1.80	0.62
1:A:734:THR:HG22	1:A:737:ALA:H	1.64	0.62
1:B:44:ASN:HD22	1:B:45:PRO:N	1.97	0.62
1:A:908:TRP:O	1:A:912:ILE:HG12	2.00	0.62
1:B:677:GLN:HB2	1:B:680:GLN:HE21	1.64	0.61
1:A:734:THR:HG23	1:A:736:GLN:HE21	1.65	0.61
1:A:179:LYS:HD2	1:A:237:VAL:HG23	1.81	0.61
1:A:708:THR:HG22	1:A:711:ARG:HD3	1.81	0.61
1:A:179:LYS:O	1:A:183:VAL:HG22	2.00	0.61
1:A:91:ASP:OD2	1:A:146:HIS:CD2	2.53	0.61
1:A:964:ASP:C	1:A:964:ASP:N	2.54	0.61
1:B:474:GLU:O	1:B:475:ASN:HB3	2.00	0.61
1:A:67:LEU:HD21	1:A:268:THR:HG23	1.83	0.61
1:A:878:THR:HG23	1:A:881:ALA:H	1.66	0.61
1:A:671:ASN:HB3	1:A:701:LYS:NZ	2.16	0.60
1:A:348:SER:OG	1:A:606:GLU:OE2	2.16	0.60
1:B:126:GLU:OE2	1:B:164:ARG:NH1	2.34	0.60
1:B:765:ARG:HH11	1:B:765:ARG:HG3	1.61	0.60
1:B:932:THR:CG2	1:B:935:ASP:H	2.14	0.60
1:B:80:ASP:OD1	1:B:82:THR:HB	2.01	0.60
1:B:829:LEU:O	1:B:852:SER:CB	2.49	0.60
1:A:711:ARG:HG2	1:A:711:ARG:NH1	2.17	0.60
1:A:635:ASN:HD21	1:A:732:ASN:HD22	1.47	0.60
1:A:354:GLY:O	1:A:380:THR:HG21	2.02	0.59
1:B:118:THR:HG21	1:B:167:GLN:HG3	1.82	0.59
1:B:558:LYS:HB3	1:B:726:GLU:HG3	1.84	0.59
1:A:47:ILE:HG21	1:A:50:ILE:HG12	1.83	0.59
1:A:297:HIS:O	1:A:477:ARG:HD2	2.03	0.59
1:A:625:TYR:CZ	1:A:765:ARG:HD2	2.38	0.58
1:B:78:ILE:HB	1:B:259:LEU:HB2	1.85	0.58
1:B:380:THR:HG22	1:B:383:GLY:N	2.06	0.58
1:B:545:THR:HG23	1:B:547:TYR:O	2.04	0.58
1:B:317:PHE:HE1	1:B:476:VAL:HG22	1.60	0.58
1:A:602:ASP:OD2	1:A:658:ARG:CD	2.51	0.58
1:B:765:ARG:CG	1:B:765:ARG:NH1	2.58	0.58
1:A:708:THR:HG21	1:A:711:ARG:HD3	1.85	0.58
1:B:934:GLU:O	1:B:938:LYS:HD2	1.98	0.58
1:B:224:TYR:CZ	1:B:229:ARG:HD2	2.39	0.57
1:A:625:TYR:CZ	1:A:765:ARG:HD3	2.40	0.57
1:A:944:LEU:O	1:A:951:ARG:NH1	2.36	0.57
1:B:789:SER:HB3	1:B:963:MET:CE	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:THR:HG21	1:B:477:ARG:HH22	1.69	0.57
1:B:111:GLN:OE1	1:B:142:THR:HG23	2.05	0.57
1:A:546:PRO:O	1:A:562:LYS:NZ	2.37	0.56
1:B:663:LYS:HD3	1:B:704:LEU:HD22	1.86	0.56
1:A:159:GLU:HG3	1:A:270:LEU:CD1	2.35	0.56
1:A:294:GLN:H	1:A:297:HIS:HD2	1.53	0.56
1:B:604:LEU:HD21	1:B:618:TYR:OH	2.05	0.56
1:A:459:PHE:CE2	1:A:461:PRO:HG3	2.41	0.56
1:A:120:LYS:NZ	1:A:163:ASP:OD2	2.39	0.56
1:A:245:HIS:O	1:A:249:TYR:HB2	2.06	0.56
1:A:349:GLU:OE1	1:A:349:GLU:HA	2.06	0.56
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.21	0.55
1:B:551:ILE:HD12	1:B:739:LEU:HD13	1.88	0.55
1:B:229:ARG:O	1:B:232:GLN:O	2.22	0.55
1:B:413:GLU:HG2	1:B:531:ILE:HD11	1.89	0.55
1:A:625:TYR:OH	1:A:765:ARG:CG	2.42	0.55
1:A:625:TYR:CZ	1:A:765:ARG:HG3	2.41	0.55
1:A:53:HIS:CE1	1:B:937:ILE:HD12	2.41	0.55
1:A:224:TYR:CZ	1:A:229:ARG:HG2	2.42	0.55
1:B:715:PHE:CE1	1:B:719:LEU:CG	2.88	0.55
1:A:97:LEU:HB2	1:A:144:GLY:O	2.07	0.55
1:B:472:ARG:O	1:B:474:GLU:O	2.25	0.55
1:B:601:LYS:CE	1:B:620:LEU:O	2.50	0.55
1:A:915:GLN:NE2	1:A:920:ARG:NH2	2.49	0.54
1:B:751:GLU:HB2	4:B:1038:HOH:O	2.06	0.54
1:B:113:MET:CE	1:B:182:GLU:CB	2.85	0.54
1:A:55:THR:CG2	1:A:451:THR:CG2	2.73	0.54
1:A:604:LEU:HD13	1:A:648:LYS:HD2	1.90	0.54
1:B:441:LEU:CD1	1:B:449:VAL:HG11	2.37	0.54
1:A:584:TYR:HB2	1:A:624:ILE:O	2.06	0.54
1:A:938:LYS:C	1:A:941:LYS:NZ	2.60	0.54
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.90	0.54
1:A:225:THR:HG22	1:A:226:LEU:HG	1.90	0.54
1:B:224:TYR:O	1:B:229:ARG:HB2	2.08	0.54
1:A:806:MET:HE1	1:A:893:ARG:HH12	1.72	0.54
1:A:858:TYR:CZ	1:A:862:ARG:HD2	2.43	0.54
1:B:795:TYR:CE1	1:B:953:LYS:HG3	2.43	0.54
1:A:541:GLU:OE2	1:A:736:GLN:NE2	2.37	0.54
1:B:415:LYS:HA	1:B:456:LEU:HD21	1.88	0.54
1:B:813:GLN:HE21	1:B:885:HIS:HD2	1.55	0.54
1:A:625:TYR:CE1	1:A:765:ARG:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:ASN:HB3	1:A:997:GLU:HB2	1.91	0.53
1:B:424:PHE:O	1:B:569:LEU:HD23	2.07	0.53
1:A:52:ASN:O	1:A:53:HIS:CB	2.56	0.53
1:B:252:ASN:O	1:B:253:LEU:HB2	2.07	0.53
1:A:625:TYR:HE1	1:A:765:ARG:HA	1.73	0.53
1:B:262:GLU:HB2	1:B:267:LEU:HD13	1.89	0.53
1:A:708:THR:HG22	1:A:711:ARG:HB2	1.91	0.53
1:A:635:ASN:HD21	1:A:732:ASN:ND2	2.06	0.53
1:B:118:THR:HG22	1:B:119:LYS:N	2.24	0.53
1:B:915:GLN:NE2	1:B:920:ARG:HH22	2.07	0.53
1:B:142:THR:CG2	1:B:147:THR:HB	2.25	0.53
1:B:591:ASN:O	1:B:595:LEU:HD22	2.09	0.53
1:B:857:HIS:HD2	4:B:1036:HOH:O	1.90	0.53
1:A:805:ASN:O	1:A:809:GLU:HG2	2.09	0.52
1:B:767:ARG:HD3	1:B:1005:PHE:O	2.09	0.52
1:B:188:SER:HB3	1:B:831:TYR:CB	2.37	0.52
1:A:55:THR:HG22	1:A:55:THR:O	2.09	0.52
1:B:600:LEU:CD1	1:B:648:LYS:HG2	2.39	0.52
1:B:86:SER:HB3	1:B:158:LEU:HG	1.91	0.52
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.40	0.52
1:B:298:LEU:HD21	1:B:318:PRO:HG2	1.91	0.52
1:B:693:VAL:HG13	1:B:766:TYR:CE1	2.44	0.52
1:B:908:TRP:O	1:B:912:ILE:HG12	2.10	0.52
2:D:3:ARG:HG2	2:D:3:ARG:NH1	2.22	0.52
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.91	0.52
1:A:118:THR:HG22	1:A:121:TYR:N	2.13	0.52
1:A:554:THR:HG22	1:A:555:ALA:N	2.25	0.52
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.92	0.52
1:B:104:ALA:O	1:B:225:THR:HG21	2.10	0.52
1:A:854:LYS:HG2	1:A:858:TYR:CD2	2.45	0.51
1:A:948:ALA:HB3	1:A:951:ARG:HB2	1.91	0.51
1:B:933:LYS:O	1:B:937:ILE:HG13	2.09	0.51
1:A:86:SER:HB3	1:A:158:LEU:HG	1.92	0.51
1:A:813:GLN:HE22	1:A:892:ARG:HH21	1.57	0.50
1:A:44:ASN:OD1	1:A:45:PRO:HD2	2.11	0.50
1:A:104:ALA:O	1:A:225:THR:HG21	2.10	0.50
1:A:676:GLU:HG3	1:A:680:GLN:OE1	2.11	0.50
1:B:677:GLN:HB3	1:B:679:HIS:CD2	2.46	0.50
1:A:196:ASN:O	1:A:200:ARG:HG2	2.12	0.50
1:B:893:ARG:NH2	1:B:921:ASP:OD1	2.44	0.50
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ASN:O	1:B:809:GLU:HB2	2.12	0.50
1:B:77:LEU:HD22	1:B:267:LEU:HB3	1.93	0.50
1:A:294:GLN:H	1:A:297:HIS:CD2	2.29	0.50
1:A:994:ASN:HD22	1:A:997:GLU:H	1.59	0.50
1:B:569:LEU:N	1:B:569:LEU:HD12	2.27	0.50
1:A:197:ASP:HA	1:A:200:ARG:HG3	1.94	0.49
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.93	0.49
1:A:554:THR:HG22	1:A:556:MET:H	1.77	0.49
1:B:932:THR:HG23	1:B:934:GLU:H	1.76	0.49
1:A:440:ILE:HD11	1:A:449:VAL:O	2.12	0.49
1:B:118:THR:CG2	1:B:119:LYS:N	2.76	0.49
1:B:854:LYS:HG2	1:B:858:TYR:CD2	2.47	0.49
1:A:380:THR:HG22	1:A:382:GLU:N	2.28	0.49
1:B:224:TYR:HA	1:B:228:THR:HB	1.93	0.49
1:A:600:LEU:HD21	1:A:648:LYS:HB3	1.95	0.49
1:B:767:ARG:HG2	1:B:1007:LEU:HD21	1.95	0.49
1:A:677:GLN:HG3	1:A:678:PRO:HD2	1.95	0.48
1:B:104:ALA:O	1:B:225:THR:HG23	2.11	0.48
1:A:224:TYR:HA	1:A:228:THR:HB	1.94	0.48
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.48	0.48
1:A:558:LYS:HB3	1:A:726:GLU:HG3	1.96	0.48
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.95	0.48
1:B:229:ARG:CB	1:B:230:PRO:HD3	2.42	0.48
1:A:559:LEU:HD22	1:A:742:MET:CG	2.43	0.48
1:B:512:LYS:HE2	1:B:512:LYS:HA	1.95	0.48
1:A:332:HIS:CE1	2:C:2:LEU:HD21	2.49	0.48
1:A:346:LEU:HA	1:A:522:PHE:CE1	2.49	0.48
1:A:460:ARG:NH2	1:A:462:ASP:OD2	2.46	0.48
1:A:409:TRP:CD1	1:B:120:LYS:HE3	2.49	0.48
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.95	0.47
1:B:155:HIS:CE1	1:B:156:GLU:HG2	2.49	0.47
1:B:793:ILE:O	1:B:847:ARG:HA	2.13	0.47
1:B:934:GLU:O	1:B:938:LYS:HD3	2.02	0.47
1:A:87:SER:HB2	1:A:151:PHE:O	2.15	0.47
1:B:715:PHE:C	1:B:715:PHE:HD1	2.16	0.47
1:A:246:SER:O	1:A:281:LYS:HD3	2.14	0.47
1:A:413:GLU:OE2	1:A:527:LYS:HE2	2.14	0.47
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.44	0.47
1:A:961:ARG:NH1	1:A:962:GLU:OE2	2.46	0.47
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.96	0.47
1:B:415:LYS:HA	1:B:456:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:TYR:CZ	1:A:765:ARG:CG	2.98	0.47
1:B:715:PHE:HE1	1:B:719:LEU:CG	2.27	0.47
1:B:44:ASN:HD22	1:B:45:PRO:CD	2.28	0.47
1:B:567:PHE:O	1:B:569:LEU:HD12	2.14	0.47
1:A:559:LEU:HD11	1:A:729:LEU:HD22	1.96	0.46
1:B:218:PHE:CE1	1:B:220:THR:HG23	2.50	0.46
1:A:64:TYR:CE1	1:A:78:ILE:HG12	2.51	0.46
1:A:346:LEU:HD22	1:A:350:LEU:HD22	1.97	0.46
1:B:299:LYS:CD	1:B:474:GLU:HA	2.45	0.46
1:A:843:ILE:HG22	1:A:844:GLN:N	2.30	0.46
1:A:47:ILE:CG2	1:A:50:ILE:HG12	2.45	0.46
1:A:625:TYR:CE2	1:A:765:ARG:HD2	2.51	0.46
1:B:119:LYS:HB3	1:B:119:LYS:HE3	1.58	0.46
1:B:765:ARG:HG2	1:B:765:ARG:NH1	2.26	0.46
1:B:932:THR:HG23	1:B:934:GLU:N	2.30	0.46
1:B:64:TYR:CE1	1:B:78:ILE:HG12	2.51	0.46
1:B:476:VAL:HG12	1:B:477:ARG:N	2.30	0.46
1:B:251:SER:C	1:B:252:ASN:O	2.51	0.45
1:B:332:HIS:CE1	2:D:2:LEU:HD11	2.51	0.45
1:B:395:PHE:HZ	1:B:476:VAL:HG21	1.80	0.45
1:B:83:THR:O	1:B:261:ARG:HD2	2.17	0.45
1:B:299:LYS:HD2	1:B:474:GLU:HA	1.97	0.45
1:A:54:ILE:HG23	1:A:446:LEU:O	2.16	0.45
1:B:232:GLN:O	1:B:233:GLU:HB2	2.15	0.45
1:B:427:LYS:HD3	1:B:898:LYS:HB3	1.97	0.45
1:A:349:GLU:OE1	1:A:521:LYS:HE2	2.17	0.45
1:B:299:LYS:HB2	1:B:299:LYS:HE3	1.71	0.45
1:A:267:LEU:O	1:A:271:VAL:HG12	2.16	0.45
1:B:418:ASN:HB3	1:B:454:TYR:O	2.17	0.45
1:A:446:LEU:O	1:A:449:VAL:HG22	2.17	0.45
1:A:551:ILE:HD12	1:A:739:LEU:HD13	1.99	0.45
1:A:179:LYS:O	1:A:183:VAL:CG2	2.64	0.44
1:A:367:ALA:O	1:A:368:ARG:C	2.55	0.44
1:A:635:ASN:HD22	1:A:732:ASN:HB3	1.82	0.44
1:A:93:HIS:NE2	1:A:368:ARG:NH1	2.66	0.44
1:B:245:HIS:O	1:B:249:TYR:HB2	2.17	0.44
1:A:313:LEU:HB3	1:A:377:VAL:HG12	2.00	0.44
2:C:3:ARG:HE	2:C:3:ARG:HB3	1.58	0.44
1:A:870:MET:HE2	1:A:870:MET:HA	1.98	0.44
1:B:751:GLU:OE2	1:B:752:HIS:CE1	2.71	0.44
1:B:685:TYR:O	1:B:689:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:ARG:HG3	1:A:1004:LEU:HB3	1.97	0.44
1:A:941:LYS:HE2	1:A:941:LYS:HB2	1.32	0.44
1:B:91:ASP:OD2	1:B:146:HIS:CD2	2.57	0.44
1:B:106:LEU:HD11	1:B:241:LEU:HD13	1.99	0.44
1:B:187:ASP:OD2	1:B:222:ASN:HB2	2.17	0.44
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.53	0.44
1:B:396:GLN:NE2	1:B:519:ASN:HD22	2.12	0.44
1:A:627:MET:HB3	1:A:628:TYR:H	1.72	0.44
1:B:559:LEU:HD22	1:B:742:MET:CG	2.48	0.44
1:B:647:GLU:O	1:B:651:THR:HB	2.18	0.44
1:B:810:LEU:HD23	1:B:936:ILE:HD11	2.00	0.44
1:A:200:ARG:HG2	1:A:200:ARG:H	1.61	0.43
1:A:584:TYR:CB	1:A:624:ILE:O	2.65	0.43
1:A:843:ILE:HG22	1:A:844:GLN:H	1.82	0.43
1:A:877:MET:HE1	1:A:882:PHE:HD1	1.82	0.43
1:A:272:VAL:O	1:A:276:SER:OG	2.33	0.43
1:A:906:LYS:NZ	1:A:921:ASP:OD1	2.49	0.43
1:A:960:ALA:HB3	1:A:963:MET:HG3	2.00	0.43
1:B:806:MET:HE1	1:B:893:ARG:NH1	2.33	0.43
1:A:708:THR:HG23	1:A:710:PRO:CD	2.41	0.43
1:B:877:MET:CE	1:B:882:PHE:HD1	2.30	0.43
1:B:982:GLN:HE21	1:B:982:GLN:HB2	1.57	0.43
1:A:110:LEU:HD23	1:A:244:PHE:CD2	2.53	0.43
1:A:744:MET:O	1:A:748:THR:CG2	2.59	0.43
1:B:191:GLU:O	1:B:194:VAL:HG22	2.17	0.43
1:B:317:PHE:CE1	1:B:476:VAL:CG2	2.88	0.43
1:A:61:LYS:HE3	1:A:61:LYS:HA	2.01	0.43
1:B:460:ARG:NH1	1:B:462:ASP:OD2	2.51	0.43
1:A:332:HIS:ND1	2:C:2:LEU:HD21	2.33	0.43
1:A:380:THR:HG22	1:A:383:GLY:H	1.84	0.43
1:A:685:TYR:OH	1:A:781:GLN:HG2	2.19	0.43
1:A:736:GLN:H	1:A:736:GLN:CD	2.22	0.43
1:B:396:GLN:NE2	1:B:519:ASN:HB2	2.33	0.43
1:A:53:HIS:NE2	1:B:875:GLU:HG2	2.33	0.42
1:B:473:PRO:HB2	1:B:514:GLN:HG3	2.01	0.42
1:A:123:LYS:HB3	1:A:126:GLU:HB2	2.01	0.42
1:A:671:ASN:HB3	1:A:701:LYS:HZ3	1.83	0.42
1:A:311:ARG:HA	1:A:481:VAL:O	2.18	0.42
1:A:635:ASN:ND2	1:A:732:ASN:HB3	2.33	0.42
1:B:78:ILE:O	1:B:259:LEU:HA	2.19	0.42
1:B:356:VAL:HG22	1:B:377:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.54	0.42
1:A:110:LEU:HD23	1:A:244:PHE:HD2	1.84	0.42
1:B:44:ASN:HD22	1:B:44:ASN:C	2.22	0.42
1:A:689:LEU:HD23	1:A:995:MET:HG2	2.00	0.42
1:B:796:GLN:HE21	1:B:843:ILE:HG21	1.84	0.42
1:A:50:ILE:HG23	1:A:67:LEU:HD12	2.01	0.42
1:A:53:HIS:HE1	1:B:937:ILE:HD12	1.83	0.42
1:A:396:GLN:NE2	1:A:519:ASN:HD22	2.17	0.42
1:B:273:LYS:HG3	1:B:274:LEU:HD13	2.02	0.42
1:B:651:THR:O	1:B:651:THR:HG22	2.19	0.42
1:B:771:LEU:HD21	1:B:954:VAL:HG12	2.02	0.42
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.55	0.41
1:B:62:ARG:HG2	1:B:80:ASP:HB2	2.02	0.41
1:B:88:ALA:HA	1:B:257:VAL:O	2.20	0.41
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.83	0.41
1:B:476:VAL:CG1	1:B:477:ARG:N	2.83	0.41
1:A:734:THR:HG22	1:A:737:ALA:CB	2.50	0.41
1:A:793:ILE:O	1:A:847:ARG:HA	2.20	0.41
1:B:75:VAL:HA	1:B:256:VAL:O	2.21	0.41
1:A:73:ILE:HG13	1:A:251:SER:HB2	2.02	0.41
1:B:121:TYR:HB3	1:B:126:GLU:HG2	2.02	0.41
1:A:243:LYS:HE2	1:A:243:LYS:HB3	1.86	0.41
1:B:120:LYS:HD3	1:B:167:GLN:NE2	2.35	0.41
1:B:151:PHE:CD1	1:B:151:PHE:C	2.94	0.41
1:B:189:GLU:HG2	1:B:831:TYR:CE1	2.55	0.41
1:B:701:LYS:HB2	1:B:701:LYS:HE3	1.85	0.41
1:B:838:ARG:HB2	1:B:847:ARG:HD3	2.02	0.41
1:B:567:PHE:O	1:B:569:LEU:CD1	2.69	0.41
1:B:630:SER:OG	1:B:632:LYS:HE2	2.20	0.41
1:B:716:ILE:HB	1:B:717:PRO:HD3	2.02	0.41
1:B:44:ASN:N	4:B:1040:HOH:O	2.53	0.41
1:B:44:ASN:HA	1:B:45:PRO:HD2	1.96	0.41
1:B:473:PRO:C	1:B:474:GLU:O	2.55	0.41
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.69	0.41
1:A:963:MET:O	1:A:964:ASP:C	2.59	0.41
1:B:425:LYS:HE3	1:B:425:LYS:HB3	1.66	0.41
1:B:789:SER:HB3	1:B:963:MET:HE2	2.02	0.41
1:A:222:ASN:H	1:A:225:THR:HB	1.86	0.41
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.96	0.41
1:A:803:SER:HA	1:A:927:TYR:CE2	2.56	0.41
1:B:697:LYS:O	1:B:701:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:SER:O	1:B:802:THR:C	2.59	0.41
1:A:52:ASN:ND2	4:A:10:HOH:O	2.46	0.41
1:A:48:LYS:NZ	4:A:11:HOH:O	2.53	0.40
1:A:139:ASN:ND2	1:A:140:ALA:H	2.19	0.40
1:A:862:ARG:NH2	1:A:981:SER:O	2.54	0.40
1:B:789:SER:HB3	1:B:963:MET:HE1	2.03	0.40
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.86	0.40
1:A:399:GLN:NE2	1:A:402:ARG:HD2	2.36	0.40
1:B:164:ARG:H	1:B:164:ARG:HG2	1.60	0.40
1:B:677:GLN:H	1:B:680:GLN:NE2	2.19	0.40
1:B:715:PHE:CE1	1:B:719:LEU:HB2	2.56	0.40
1:A:56:LYS:HD2	1:A:60:ASP:HB3	2.03	0.40
1:A:346:LEU:HD11	1:A:394:MET:HG2	2.03	0.40
1:A:599:LEU:HD23	1:A:662:ILE:HD12	2.02	0.40
1:B:192:LYS:HE2	1:B:192:LYS:HB3	1.79	0.40
1:A:53:HIS:C	1:A:54:ILE:HD13	2.41	0.40
1:A:686:LEU:HD22	1:A:690:MET:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	950/990 (96%)	915 (96%)	35 (4%)	0	100	100
1	B	949/990 (96%)	913 (96%)	36 (4%)	0	100	100
2	C	1/28 (4%)	1 (100%)	0	0	100	100
2	D	1/28 (4%)	1 (100%)	0	0	100	100
All	All	1901/2036 (93%)	1830 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	849/879 (97%)	740 (87%)	109 (13%)	4 18
1	B	849/879 (97%)	744 (88%)	105 (12%)	4 19
2	C	3/22 (14%)	2 (67%)	1 (33%)	0 1
2	D	3/22 (14%)	3 (100%)	0	100 100
All	All	1704/1802 (95%)	1489 (87%)	215 (13%)	4 18

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	50	ILE
1	A	53	HIS
1	A	55	THR
1	A	61	LYS
1	A	69	LEU
1	A	83	THR
1	A	84	ASP
1	A	87	SER
1	A	97	LEU
1	A	106	LEU
1	A	110	LEU
1	A	118	THR
1	A	139	ASN
1	A	143	SER
1	A	145	GLU
1	A	158	LEU
1	A	162	LEU
1	A	173	LEU
1	A	183	VAL
1	A	188	SER
1	A	200	ARG
1	A	201	LEU
1	A	204	LEU

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Mol	Chain	Res	Type
1	A	225	THR
1	A	229	ARG
1	A	242	LEU
1	A	264	LEU
1	A	267	LEU
1	A	281	LYS
1	A	285	LEU
1	A	295	GLU
1	A	296	GLU
1	A	346	LEU
1	A	348	SER
1	A	350	LEU
1	A	358	THR
1	A	368	ARG
1	A	377	VAL
1	A	380	THR
1	A	385	LEU
1	A	392	LEU
1	A	420	VAL
1	A	423	ARG
1	A	450	LEU
1	A	454	TYR
1	A	458	GLU
1	A	471	LEU
1	A	508	GLU
1	A	524	LEU
1	A	527	LYS
1	A	529	GLU
1	A	533	THR
1	A	558	LYS
1	A	562	LYS
1	A	566	LYS
1	A	569	LEU
1	A	574	LEU
1	A	590	SER
1	A	600	LEU
1	A	613	LEU
1	A	641	LEU
1	A	648	LYS
1	A	664	GLU
1	A	669	SER
1	A	671	ASN

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Mol	Chain	Res	Type
1	A	674	ARG
1	A	676	GLU
1	A	677	GLN
1	A	686	LEU
1	A	691	THR
1	A	697	LYS
1	A	704	LEU
1	A	708	THR
1	A	709	LEU
1	A	711	ARG
1	A	719	LEU
1	A	720	LEU
1	A	723	LEU
1	A	729	LEU
1	A	734	THR
1	A	736	GLN
1	A	739	LEU
1	A	742	MET
1	A	748	THR
1	A	759	LEU
1	A	765	ARG
1	A	767	ARG
1	A	771	LEU
1	A	782	ARG
1	A	792	GLU
1	A	810	LEU
1	A	847	ARG
1	A	859	LEU
1	A	863	VAL
1	A	872	LYS
1	A	875	GLU
1	A	889	LEU
1	A	896	LYS
1	A	901	SER
1	A	906	LYS
1	A	914	GLN
1	A	933	LYS
1	A	934	GLU
1	A	941	LYS
1	A	946	VAL
1	A	982	GLN
1	A	1002	LEU

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Mol	Chain	Res	Type
1	A	1009	LYS
1	B	44	ASN
1	B	55	THR
1	B	61	LYS
1	B	69	LEU
1	B	147	THR
1	B	158	LEU
1	B	162	LEU
1	B	164	ARG
1	B	167	GLN
1	B	179	LYS
1	B	186	VAL
1	B	188	SER
1	B	192	LYS
1	B	201	LEU
1	B	220	THR
1	B	225	THR
1	B	229	ARG
1	B	239	GLN
1	B	241	LEU
1	B	259	LEU
1	B	264	LEU
1	B	267	LEU
1	B	273	LYS
1	B	274	LEU
1	B	276	SER
1	B	277	GLU
1	B	287	GLU
1	B	299	LYS
1	B	301	LEU
1	B	305	VAL
1	B	334	LEU
1	B	346	LEU
1	B	358	THR
1	B	360	VAL
1	B	364	LYS
1	B	377	VAL
1	B	380	THR
1	B	401	LEU
1	B	414	LEU
1	B	446	LEU
1	B	447	GLU

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Mol	Chain	Res	Type
1	B	456	LEU
1	B	463	LEU
1	B	466	MET
1	B	471	LEU
1	B	508	GLU
1	B	512	LYS
1	B	518	LEU
1	B	523	LYS
1	B	526	THR
1	B	529	GLU
1	B	566	LYS
1	B	603	SER
1	B	604	LEU
1	B	613	LEU
1	B	641	LEU
1	B	642	LEU
1	B	644	LYS
1	B	663	LYS
1	B	669	SER
1	B	677	GLN
1	B	693	VAL
1	B	697	LYS
1	B	704	LEU
1	B	708	THR
1	B	712	LEU
1	B	715	PHE
1	B	719	LEU
1	B	728	LEU
1	B	736	GLN
1	B	739	LEU
1	B	742	MET
1	B	744	MET
1	B	749	LEU
1	B	759	LEU
1	B	765	ARG
1	B	769	VAL
1	B	771	LEU
1	B	788	ASN
1	B	808	LEU
1	B	809	GLU
1	B	817	GLU
1	B	829	LEU

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Mol	Chain	Res	Type
1	B	838	ARG
1	B	853	GLU
1	B	859	LEU
1	B	873	SER
1	B	880	GLU
1	B	889	LEU
1	B	898	LYS
1	B	901	SER
1	B	914	GLN
1	B	932	THR
1	B	934	GLU
1	B	938	LYS
1	B	942	GLU
1	B	951	ARG
1	B	954	VAL
1	B	959	LEU
1	B	962	GLU
1	B	980	LEU
1	B	982	GLN
1	B	986	LEU
1	B	991	VAL
1	B	1002	LEU
2	C	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	146	HIS
1	A	231	ASN
1	A	297	HIS
1	A	357	ASN
1	A	396	GLN
1	A	399	GLN
1	A	502	GLN
1	A	514	GLN
1	A	732	ASN
1	A	780	GLN
1	A	786	HIS
1	A	787	ASN
1	A	796	GLN
1	A	800	GLN

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Mol	Chain	Res	Type
1	A	813	GLN
1	A	828	GLN
1	A	885	HIS
1	A	887	GLN
1	A	915	GLN
1	A	982	GLN
1	A	994	ASN
1	B	44	ASN
1	B	146	HIS
1	B	148	ASN
1	B	157	HIS
1	B	167	GLN
1	B	196	ASN
1	B	203	GLN
1	B	231	ASN
1	B	232	GLN
1	B	300	GLN
1	B	363	GLN
1	B	396	GLN
1	B	399	GLN
1	B	418	ASN
1	B	499	GLN
1	B	635	ASN
1	B	671	ASN
1	B	679	HIS
1	B	680	GLN
1	B	780	GLN
1	B	786	HIS
1	B	788	ASN
1	B	800	GLN
1	B	805	ASN
1	B	857	HIS
1	B	885	HIS
1	B	915	GLN
1	B	982	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	954/990 (96%)	-0.56	4 (0%)	92	79	28, 41, 54, 68	0
1	B	953/990 (96%)	-0.58	2 (0%)	95	87	24, 38, 51, 63	0
2	C	3/28 (10%)	-0.11	0	100	100	64, 64, 66, 69	0
2	D	3/28 (10%)	0.09	0	100	100	66, 66, 67, 70	0
All	All	1913/2036 (93%)	-0.57	6 (0%)	94	83	24, 39, 52, 70	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	ASN	3.0
1	B	1011	HIS	2.7
1	A	53	HIS	2.6
1	B	543	GLU	2.1
1	A	45	PRO	2.0
1	A	1011	HIS	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
3	ZN	A	1	1/1	0.93	0.12	63,63,63,63	0
3	ZN	B	2	1/1	0.96	0.18	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.