Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 11:59 PM EDT

PDB ID	:	3MRU
Title	:	Crystal Structure of Aminoacylhistidine Dipeptidase from Vibrio alginolyticus
Authors	:	Chang, C.-Y.; Hsieh, Y.-C.; Wu, T.-K.; Chen, C.-J.
Deposited on	:	2010-04-29
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

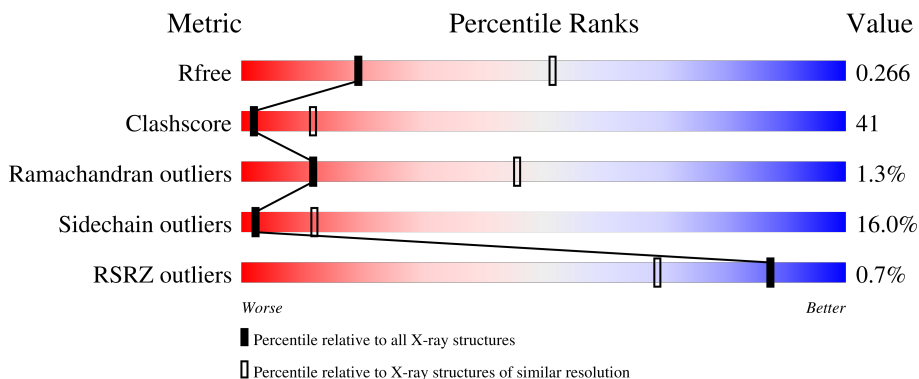|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		41
Ramachandran outliers		1.3%
Sidechain outliers		16.0%
RSRZ outliers		0.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	490	51% 38% 10% •
1	B	490	.% 49% 40% 10% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7530 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 Aminoacyl-histidine dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3763	2383	626	731	23			
1	B	490	Total	C	N	O	S	0	0	0
			3763	2383	626	731	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots ⓘ

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: Aminoacyl-histidine dipeptidase

Chain A:

• Molecule 1: Aminoacyl-histidine dipeptidase

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	80.41Å 80.41Å 303.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.57 – 3.00 27.57 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.9 (27.57-3.00) 99.9 (27.57-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.80Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.231 , 0.273 0.239 , 0.266	Depositor DCC
R_{free} test set	1385 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.0	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7530	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.62	0/3841	0.82	8/5206 (0.2%)
1	B	0.61	0/3841	0.86	11/5206 (0.2%)
All	All	0.61	0/7682	0.84	19/10412 (0.2%)

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

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

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	ALA	CB-CA-C	-9.09	96.47	110.10
1	B	453	PHE	CB-CA-C	-8.38	93.63	110.40
1	B	3	GLU	N-CA-C	-8.36	88.42	111.00
1	A	28	HIS	N-CA-CB	-7.15	97.73	110.60
1	B	423	TYR	CB-CA-C	6.89	124.18	110.40
1	B	312	ASP	N-CA-C	6.63	128.91	111.00
1	B	488	GLU	N-CA-C	6.46	128.46	111.00
1	B	161	ALA	CB-CA-C	6.02	119.13	110.10
1	A	56	THR	CB-CA-C	-6.00	95.41	111.60
1	A	342	VAL	N-CA-C	5.85	126.79	111.00
1	B	311	THR	N-CA-C	5.81	126.69	111.00
1	B	487	PRO	CB-CA-C	-5.80	97.50	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	VAL	CB-CA-C	-5.75	100.47	111.40
1	B	28	HIS	N-CA-CB	-5.74	100.27	110.60
1	A	57	GLY	N-CA-C	5.72	127.41	113.10
1	A	453	PHE	CB-CA-C	-5.48	99.44	110.40
1	B	487	PRO	O-C-N	-5.45	113.97	122.70
1	B	446	PRO	CB-CA-C	-5.38	98.56	112.00
1	A	169	LEU	CA-CB-CG	5.09	127.00	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	423	TYR	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	VAL	Peptide
1	B	487	PRO	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	3763	0	3696	299	0
1	B	3763	0	3696	308	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	7530	0	7392	605	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 41.

All (605) 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:486:ILE:CD1	1:B:487:PRO:HD2	1.48	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ILE:HG12	1:B:467:VAL:CG1	1.54	1.36
1:B:486:ILE:HD13	1:B:487:PRO:CD	1.54	1.36
1:B:443:GLU:CG	1:B:444:PRO:HD3	1.64	1.28
1:B:488:GLU:O	1:B:489:LYS:HD2	1.34	1.27
1:B:443:GLU:OE1	1:B:444:PRO:HD3	1.35	1.27
1:A:312:ASP:HA	1:A:313:ALA:CB	1.65	1.26
1:B:443:GLU:CD	1:B:444:PRO:HD3	1.55	1.25
1:A:122:ILE:CG2	1:A:455:PRO:HG3	1.72	1.18
1:B:254:ARG:NH2	1:B:356:THR:HG22	1.59	1.15
1:A:87:LYS:HD2	1:A:87:LYS:N	1.50	1.15
1:B:443:GLU:OE1	1:B:444:PRO:CD	1.96	1.14
1:B:69:MET:HB2	1:B:72:LYS:HG2	1.24	1.14
1:B:457:ILE:CG1	1:B:467:VAL:HG12	1.78	1.13
1:B:457:ILE:HG23	1:B:467:VAL:HG13	1.32	1.12
1:A:87:LYS:H	1:A:87:LYS:CD	1.64	1.11
1:B:188:ILE:HD13	1:B:399:ALA:HB2	1.34	1.09
1:A:443:GLU:HB3	1:A:444:PRO:HD3	1.22	1.09
1:B:168:ILE:HD12	1:B:449:ASP:HB3	1.34	1.08
1:A:87:LYS:O	1:A:87:LYS:HD3	1.54	1.06
1:A:457:ILE:HG13	1:A:467:VAL:CG1	1.88	1.04
1:A:457:ILE:CG1	1:A:467:VAL:HG13	1.88	1.04
1:A:120:ASN:O	1:A:123:GLY:N	1.90	1.03
1:A:122:ILE:HG21	1:A:455:PRO:CG	1.89	1.03
1:B:159:LEU:C	1:B:160:GLU:HG3	1.72	1.02
1:A:312:ASP:HA	1:A:313:ALA:HB2	1.04	1.02
1:B:335:VAL:CG1	1:B:346:VAL:HG13	1.92	1.00
1:A:161:ALA:HA	1:A:445:TYR:CZ	1.96	1.00
1:A:122:ILE:HG21	1:A:455:PRO:HG3	1.01	0.99
1:A:207:THR:OG1	1:A:310:ALA:HA	1.62	0.99
1:A:112:LYS:HE3	1:A:112:LYS:HA	1.45	0.98
1:A:159:LEU:H	1:A:159:LEU:HD22	1.26	0.98
1:B:457:ILE:HG12	1:B:467:VAL:HG12	1.00	0.97
1:B:334:GLY:O	1:B:336:MET:CE	2.13	0.97
1:B:422:ILE:HG13	1:B:422:ILE:O	1.63	0.96
1:A:284:PHE:O	1:A:288:THR:HG22	1.66	0.96
1:B:443:GLU:CG	1:B:444:PRO:CD	2.43	0.96
1:A:26:ILE:HD11	1:A:36:LEU:HD22	1.47	0.95
1:A:457:ILE:HG13	1:A:467:VAL:HG13	0.96	0.95
1:B:88:ASN:O	1:B:91:THR:HG22	1.66	0.95
1:A:221:GLY:O	1:A:433:HIS:HB3	1.67	0.95
1:B:426:LYS:HG2	1:B:427:PRO:HD2	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASP:OD1	1:A:151:ALA:HB3	1.68	0.93
1:B:71:ASN:H	1:B:71:ASN:ND2	1.67	0.93
1:B:257:SER:OG	1:B:258:LEU:N	1.92	0.92
1:B:334:GLY:O	1:B:336:MET:HE3	1.69	0.92
1:A:456:THR:CG2	1:A:471:THR:HG21	1.98	0.92
1:B:161:ALA:HA	1:B:445:TYR:CZ	2.05	0.92
1:B:254:ARG:HH22	1:B:356:THR:HG22	1.29	0.92
1:B:23:ILE:HD13	1:B:36:LEU:HD11	1.50	0.91
1:A:51:VAL:HG22	1:A:61:ILE:HG12	1.51	0.90
1:B:443:GLU:HG2	1:B:444:PRO:HD3	1.54	0.90
1:A:201:ILE:HD11	1:A:313:ALA:HB1	1.54	0.90
1:B:335:VAL:HG13	1:B:346:VAL:HG13	1.54	0.89
1:B:460:PRO:HB2	1:B:461:HIS:HD2	1.36	0.89
1:B:71:ASN:C	1:B:488:GLU:HB2	1.93	0.89
1:A:443:GLU:HB3	1:A:444:PRO:CD	2.02	0.89
1:B:441:PHE:O	1:B:444:PRO:O	1.91	0.89
1:B:226:THR:HB	1:B:228:ARG:HG2	1.56	0.88
1:B:71:ASN:H	1:B:71:ASN:HD22	1.19	0.88
1:A:312:ASP:CA	1:A:313:ALA:CB	2.49	0.88
1:A:87:LYS:HD2	1:A:87:LYS:H	0.75	0.88
1:A:208:ARG:NE	1:A:308:GLU:HB3	1.88	0.88
1:A:318:ILE:HD12	1:A:322:GLN:HG3	1.56	0.87
1:B:335:VAL:HG13	1:B:346:VAL:CG1	2.05	0.86
1:B:488:GLU:O	1:B:489:LYS:CD	2.22	0.86
1:A:75:VAL:HG21	1:A:486:ILE:HD13	1.58	0.86
1:A:87:LYS:N	1:A:87:LYS:CD	2.30	0.85
1:B:16:LEU:HD21	1:B:122:ILE:HG23	1.57	0.85
1:B:262:ILE:HD13	1:B:351:ASN:ND2	1.90	0.85
1:A:159:LEU:HD22	1:A:159:LEU:N	1.90	0.85
1:B:188:ILE:HD13	1:B:399:ALA:CB	2.06	0.84
1:A:249:ARG:HB3	1:A:315:VAL:HG11	1.57	0.84
1:A:312:ASP:CA	1:A:313:ALA:HB2	2.00	0.83
1:A:455:PRO:HG2	1:A:457:ILE:HD11	1.59	0.83
1:A:26:ILE:CD1	1:A:36:LEU:HD13	2.09	0.83
1:A:188:ILE:HD13	1:A:189:ASP:O	1.80	0.82
1:B:359:GLU:CD	1:B:359:GLU:H	1.83	0.82
1:A:208:ARG:HE	1:A:308:GLU:HB3	1.43	0.82
1:A:56:THR:O	1:A:56:THR:OG1	1.92	0.81
1:B:71:ASN:HB2	1:B:488:GLU:HB2	1.63	0.81
1:B:311:THR:HG22	1:B:311:THR:O	1.79	0.81
1:B:457:ILE:CG2	1:B:467:VAL:HG13	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASN:HD22	1:A:488:GLU:HB2	1.45	0.80
1:B:183:GLY:HA2	1:B:403:TRP:CD2	2.17	0.79
1:B:285:ASN:HA	1:B:288:THR:HG22	1.65	0.79
1:A:87:LYS:CD	1:A:87:LYS:O	2.30	0.79
1:B:422:ILE:O	1:B:422:ILE:CG1	2.30	0.79
1:B:87:LYS:HB2	1:B:91:THR:HG21	1.63	0.78
1:B:75:VAL:HG22	1:B:141:ILE:HD13	1.63	0.78
1:B:457:ILE:HG12	1:B:467:VAL:HG11	1.65	0.78
1:A:26:ILE:HD13	1:A:26:ILE:O	1.83	0.78
1:B:168:ILE:CD1	1:B:449:ASP:HB3	2.12	0.78
1:A:88:ASN:HB2	1:A:113:GLY:HA2	1.66	0.77
1:B:16:LEU:HD21	1:B:122:ILE:CG2	2.14	0.77
1:B:457:ILE:CG1	1:B:467:VAL:CG1	2.46	0.77
1:A:211:THR:HG23	1:A:305:PHE:HB2	1.66	0.77
1:B:232:ASN:CG	1:B:355:ILE:HD13	2.05	0.77
1:A:118:ALA:CB	1:A:467:VAL:HG21	2.14	0.77
1:B:443:GLU:HG2	1:B:444:PRO:CD	2.11	0.77
1:A:288:THR:HB	1:A:304:THR:HG21	1.67	0.76
1:B:230:ASN:HD21	1:B:232:ASN:HB2	1.51	0.76
1:A:171:ASN:ND2	1:A:173:ASP:H	1.82	0.76
1:A:230:ASN:HD21	1:A:232:ASN:HB2	1.51	0.75
1:B:161:ALA:HA	1:B:445:TYR:CE2	2.21	0.75
1:A:159:LEU:H	1:A:159:LEU:CD2	1.99	0.75
1:A:299:GLU:CB	1:A:302:ILE:HD11	2.16	0.75
1:B:250:LEU:H	1:B:321:GLN:NE2	1.85	0.75
1:B:457:ILE:HG23	1:B:467:VAL:CG1	2.14	0.75
1:A:188:ILE:HD11	1:A:396:PHE:HB3	1.69	0.74
1:B:8:ILE:H	1:B:8:ILE:HD12	1.53	0.74
1:B:176:GLN:HB3	1:B:179:GLU:HG2	1.70	0.74
1:A:26:ILE:HD11	1:A:36:LEU:CD2	2.17	0.74
1:A:299:GLU:HB2	1:A:302:ILE:HD11	1.69	0.74
1:B:206:ILE:HD13	1:B:207:THR:N	2.03	0.74
1:A:87:LYS:HD3	1:A:87:LYS:C	2.07	0.74
1:A:456:THR:HG22	1:A:471:THR:HG21	1.69	0.74
1:B:423:TYR:CD1	1:B:424:GLY:O	2.41	0.74
1:A:41:VAL:HG12	1:A:51:VAL:HG11	1.71	0.73
1:B:182:MET:HB3	1:B:412:MET:HE3	1.71	0.73
1:A:26:ILE:HD12	1:A:36:LEU:HD13	1.71	0.73
1:B:488:GLU:C	1:B:489:LYS:HD2	2.09	0.73
1:A:212:LEU:HB3	1:A:235:ILE:HD11	1.68	0.73
1:B:71:ASN:O	1:B:488:GLU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ASN:O	1:B:489:LYS:N	2.21	0.73
1:B:443:GLU:CB	1:B:444:PRO:CD	2.66	0.72
1:A:171:ASN:HD21	1:A:173:ASP:HB3	1.54	0.72
1:A:438:CYS:HA	1:A:441:PHE:CD1	2.23	0.72
1:B:334:GLY:O	1:B:336:MET:HE2	1.88	0.72
1:A:456:THR:HG21	1:A:471:THR:HG21	1.71	0.72
1:B:159:LEU:O	1:B:160:GLU:HG3	1.90	0.72
1:B:58:ASN:OD1	1:B:147:ILE:HD13	1.89	0.72
1:B:262:ILE:HD13	1:B:351:ASN:HD22	1.52	0.72
1:A:208:ARG:NH2	1:A:306:ASN:O	2.23	0.72
1:A:342:VAL:HG12	1:A:342:VAL:O	1.88	0.72
1:B:206:ILE:HD12	1:B:208:ARG:HG3	1.72	0.72
1:B:120:ASN:HB3	1:B:123:GLY:HA3	1.71	0.71
1:B:413:ALA:O	1:B:417:ASP:OD1	2.07	0.71
1:B:184:CYS:HB2	1:B:434:ALA:O	1.91	0.71
1:B:332:PRO:O	1:B:350:LEU:HD21	1.90	0.71
1:A:455:PRO:HG2	1:A:457:ILE:CD1	2.20	0.71
1:A:161:ALA:HA	1:A:445:TYR:OH	1.91	0.70
1:B:211:THR:HG23	1:B:305:PHE:HB2	1.72	0.70
1:A:171:ASN:HD21	1:A:173:ASP:CB	2.04	0.70
1:B:335:VAL:HG11	1:B:346:VAL:HG13	1.73	0.70
1:B:158:GLY:O	1:B:159:LEU:HB2	1.91	0.69
1:A:159:LEU:N	1:A:159:LEU:CD2	2.55	0.69
1:A:411:ILE:HD12	1:A:451:VAL:HG21	1.74	0.69
1:B:332:PRO:HG3	1:B:382:MET:HE2	1.73	0.69
1:B:23:ILE:CD1	1:B:36:LEU:HD11	2.20	0.69
1:A:148:ASP:O	1:A:153:MET:HA	1.93	0.69
1:A:28:HIS:CE1	1:A:83:MET:HE1	2.27	0.69
1:A:41:VAL:HG12	1:A:51:VAL:CG1	2.22	0.69
1:A:87:LYS:CD	1:A:87:LYS:C	2.61	0.69
1:A:73:LYS:HG3	1:A:486:ILE:CG2	2.22	0.69
1:B:188:ILE:HD12	1:B:397:SER:O	1.93	0.68
1:B:257:SER:OG	1:B:258:LEU:HG	1.92	0.68
1:A:124:MET:HE3	1:A:145:LEU:HD22	1.76	0.68
1:B:468:LYS:HB3	1:B:471:THR:HG23	1.76	0.68
1:B:423:TYR:CE1	1:B:424:GLY:O	2.47	0.68
1:A:20:PHE:HE1	1:A:121:GLY:HA3	1.59	0.67
1:B:443:GLU:CB	1:B:444:PRO:HD3	2.25	0.67
1:B:75:VAL:HG22	1:B:141:ILE:CD1	2.25	0.67
1:A:416:ARG:HG2	1:A:426:LYS:HD3	1.77	0.67
1:B:206:ILE:HD12	1:B:208:ARG:CG	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:HB3	1:A:123:GLY:HA3	1.78	0.66
1:A:76:VAL:HB	1:A:169:LEU:HD22	1.78	0.66
1:B:208:ARG:NH2	1:B:306:ASN:O	2.29	0.66
1:B:254:ARG:HH22	1:B:356:THR:CG2	2.06	0.66
1:B:456:THR:OG1	1:B:471:THR:HG21	1.95	0.66
1:B:69:MET:HB2	1:B:72:LYS:CG	2.15	0.66
1:A:26:ILE:CD1	1:A:36:LEU:HD22	2.25	0.66
1:A:167:ASP:HA	1:A:448:MET:HG2	1.76	0.66
1:B:159:LEU:O	1:B:160:GLU:CG	2.44	0.66
1:A:100:ILE:HD12	1:A:100:ILE:H	1.61	0.66
1:B:159:LEU:C	1:B:160:GLU:CG	2.55	0.65
1:B:167:ASP:C	1:B:168:ILE:HD13	2.16	0.65
1:A:71:ASN:ND2	1:A:488:GLU:HB2	2.11	0.65
1:B:206:ILE:CD1	1:B:208:ARG:HG3	2.25	0.65
1:A:75:VAL:CG2	1:A:486:ILE:HD13	2.25	0.65
1:B:119:ASP:OD1	1:B:120:ASN:ND2	2.29	0.65
1:A:120:ASN:O	1:A:122:ILE:N	2.30	0.65
1:B:100:ILE:HD12	1:B:100:ILE:H	1.62	0.65
1:A:120:ASN:C	1:A:123:GLY:H	1.99	0.65
1:B:354:VAL:C	1:B:355:ILE:HD12	2.17	0.65
1:A:196:ILE:O	1:A:360:ASN:HA	1.98	0.64
1:A:26:ILE:HD11	1:A:36:LEU:HD13	1.78	0.64
1:B:188:ILE:CD1	1:B:399:ALA:HB2	2.21	0.64
1:A:71:ASN:HD22	1:A:488:GLU:CB	2.11	0.64
1:B:182:MET:HB3	1:B:412:MET:CE	2.27	0.64
1:B:347:GLU:CG	1:B:372:ILE:HD13	2.27	0.64
1:B:443:GLU:OE1	1:B:444:PRO:CG	2.45	0.64
1:B:453:PHE:CG	1:B:453:PHE:O	2.51	0.64
1:A:119:ASP:C	1:A:119:ASP:OD1	2.37	0.63
1:B:119:ASP:OD1	1:B:119:ASP:C	2.37	0.63
1:B:416:ARG:HG3	1:B:417:ASP:OD1	1.99	0.63
1:A:20:PHE:CE1	1:A:121:GLY:HA3	2.33	0.63
1:B:23:ILE:HD12	1:B:36:LEU:HD21	1.80	0.63
1:B:168:ILE:HD12	1:B:449:ASP:CB	2.22	0.63
1:A:120:ASN:C	1:A:122:ILE:N	2.50	0.63
1:B:54:ASP:HB2	1:B:55:PRO:HD2	1.81	0.63
1:B:66:THR:OG1	1:B:137:LYS:HA	1.99	0.62
1:A:198:ARG:HB3	1:A:314:GLN:HB3	1.81	0.62
1:A:212:LEU:CB	1:A:235:ILE:HD11	2.29	0.62
1:A:418:MET:SD	1:A:418:MET:C	2.77	0.62
1:A:89:GLU:O	1:A:90:ASP:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:CYS:HB2	1:A:434:ALA:O	2.00	0.62
1:B:285:ASN:HA	1:B:288:THR:CG2	2.30	0.62
1:A:73:LYS:O	1:A:74:GLY:O	2.18	0.62
1:A:148:ASP:OD2	1:A:151:ALA:O	2.18	0.62
1:A:44:ALA:HB3	1:A:51:VAL:HG21	1.82	0.62
1:A:470:ASP:OD1	1:A:470:ASP:N	2.32	0.61
1:B:148:ASP:O	1:B:153:MET:HA	2.00	0.61
1:A:72:LYS:O	1:A:73:LYS:HB2	2.01	0.61
1:A:416:ARG:NE	1:A:429:ILE:HD12	2.15	0.61
1:A:84:VAL:HG22	1:A:150:GLU:HG2	1.81	0.61
1:B:176:GLN:HB3	1:B:179:GLU:CG	2.30	0.61
1:B:177:GLU:HB3	1:B:456:THR:HG23	1.83	0.61
1:B:460:PRO:HB2	1:B:461:HIS:CD2	2.25	0.61
1:A:33:GLU:HG3	1:A:147:ILE:HG13	1.82	0.61
1:A:176:GLN:HB3	1:A:179:GLU:HB2	1.83	0.61
1:A:83:MET:HG2	1:A:84:VAL:N	2.16	0.61
1:B:249:ARG:HA	1:B:321:GLN:HE22	1.66	0.61
1:A:30:SER:HA	1:A:82:ASP:HB2	1.82	0.61
1:A:254:ARG:HH11	1:A:357:THR:H	1.48	0.61
1:B:196:ILE:HG22	1:B:320:ASP:HB3	1.83	0.61
1:B:448:MET:O	1:B:450:MET:HG2	2.01	0.61
1:B:335:VAL:CG1	1:B:346:VAL:CG1	2.68	0.60
1:B:418:MET:HA	1:B:418:MET:CE	2.30	0.60
1:B:84:VAL:HG22	1:B:150:GLU:HG2	1.83	0.60
1:B:482:LEU:HA	1:B:485:ALA:HB3	1.84	0.60
1:A:188:ILE:CD1	1:A:189:ASP:O	2.49	0.60
1:A:180:VAL:HG12	1:A:451:VAL:HG12	1.84	0.60
1:A:188:ILE:HD13	1:A:189:ASP:N	2.17	0.60
1:A:201:ILE:HD11	1:A:313:ALA:CB	2.29	0.60
1:A:312:ASP:HA	1:A:313:ALA:HB3	1.77	0.60
1:A:454:GLY:HA2	1:A:475:PHE:CD2	2.36	0.60
1:B:156:ALA:HB1	1:B:440:LEU:HB2	1.82	0.60
1:B:246:LEU:HD11	1:B:280:LEU:HB2	1.83	0.60
1:A:150:GLU:O	1:A:150:GLU:HG3	2.01	0.60
1:B:30:SER:HA	1:B:82:ASP:HB2	1.83	0.60
1:B:412:MET:CE	1:B:451:VAL:HG12	2.32	0.59
1:B:220:SER:O	1:B:224:ILE:HB	2.01	0.59
1:A:372:ILE:HG22	1:A:374:SER:HB3	1.82	0.59
1:A:52:ARG:HD3	1:A:60:PHE:HB2	1.84	0.59
1:A:123:GLY:O	1:A:126:SER:HB3	2.00	0.59
1:B:272:LEU:HD13	1:B:280:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ASP:OD1	1:B:323:ARG:NH1	2.35	0.59
1:B:426:LYS:HG2	1:B:427:PRO:CD	2.29	0.59
1:B:83:MET:HG2	1:B:84:VAL:N	2.17	0.59
1:B:411:ILE:HD12	1:B:412:MET:N	2.18	0.59
1:B:443:GLU:HG2	1:B:444:PRO:N	2.11	0.59
1:A:52:ARG:HD2	1:A:52:ARG:N	2.16	0.59
1:A:299:GLU:HB3	1:A:302:ILE:HD11	1.85	0.59
1:B:71:ASN:C	1:B:488:GLU:CB	2.68	0.59
1:B:468:LYS:HB3	1:B:471:THR:CG2	2.32	0.59
1:B:169:LEU:HB3	1:B:450:MET:HB3	1.85	0.59
1:B:71:ASN:ND2	1:B:71:ASN:N	2.43	0.59
1:A:58:ASN:OD1	1:A:146:THR:HA	2.03	0.58
1:B:488:GLU:CD	1:B:488:GLU:N	2.56	0.58
1:A:159:LEU:C	1:A:159:LEU:HD23	2.23	0.58
1:B:66:THR:HG23	1:B:138:HIS:CD2	2.38	0.58
1:A:138:HIS:CD2	1:A:141:ILE:HD12	2.38	0.58
1:B:486:ILE:HD13	1:B:487:PRO:HD2	0.65	0.58
1:A:169:LEU:HB3	1:A:450:MET:HB3	1.84	0.58
1:A:81:ILE:HD12	1:A:147:ILE:CD1	2.33	0.58
1:B:206:ILE:HD13	1:B:207:THR:C	2.23	0.58
1:B:206:ILE:HD13	1:B:207:THR:O	2.03	0.58
1:A:34:GLU:O	1:A:35:ALA:HB2	2.04	0.58
1:A:456:THR:HG22	1:A:471:THR:CG2	2.34	0.58
1:B:87:LYS:HB2	1:B:91:THR:CG2	2.32	0.58
1:B:179:GLU:HA	1:B:428:ASN:O	2.03	0.58
1:A:208:ARG:NH1	1:A:277:GLN:HE21	2.02	0.58
1:A:36:LEU:O	1:A:40:ILE:HG12	2.03	0.57
1:B:369:ARG:HG2	1:B:369:ARG:HH11	1.69	0.57
1:A:75:VAL:HG21	1:A:486:ILE:CD1	2.33	0.57
1:A:112:LYS:HA	1:A:112:LYS:CE	2.22	0.57
1:A:119:ASP:OD1	1:A:120:ASN:ND2	2.38	0.57
1:B:118:ALA:HB1	1:B:467:VAL:HG11	1.87	0.57
1:A:335:VAL:HG13	1:A:346:VAL:HG13	1.86	0.57
1:B:198:ARG:HB3	1:B:314:GLN:HB2	1.87	0.57
1:B:196:ILE:O	1:B:360:ASN:HA	2.04	0.57
1:B:335:VAL:HG13	1:B:346:VAL:HG11	1.87	0.57
1:B:80:HIS:CE1	1:B:82:ASP:O	2.57	0.56
1:A:201:ILE:CD1	1:A:313:ALA:HB1	2.32	0.56
1:A:348:THR:HG23	1:A:370:SER:HB2	1.87	0.56
1:B:124:MET:CE	1:B:145:LEU:HD13	2.36	0.56
1:B:71:ASN:CB	1:B:488:GLU:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LYS:HD2	1:B:91:THR:HG23	1.87	0.56
1:B:90:ASP:OD1	1:B:90:ASP:N	2.30	0.56
1:B:188:ILE:HD13	1:B:399:ALA:CA	2.35	0.56
1:A:230:ASN:ND2	1:A:232:ASN:HB2	2.20	0.56
1:A:26:ILE:CD1	1:A:26:ILE:O	2.52	0.56
1:B:180:VAL:HG21	1:B:415:PHE:CE1	2.39	0.56
1:A:26:ILE:HD11	1:A:36:LEU:CG	2.35	0.56
1:B:206:ILE:CD1	1:B:208:ARG:CG	2.83	0.56
1:A:8:ILE:HD13	1:A:104:ILE:HG13	1.87	0.55
1:A:230:ASN:HD22	1:A:233:LYS:H	1.53	0.55
1:B:232:ASN:ND2	1:B:355:ILE:HD13	2.21	0.55
1:B:355:ILE:HD12	1:B:355:ILE:N	2.22	0.55
1:A:254:ARG:HE	1:A:356:THR:HA	1.72	0.55
1:B:87:LYS:HD2	1:B:91:THR:CG2	2.37	0.55
1:B:230:ASN:HD22	1:B:233:LYS:H	1.54	0.55
1:A:73:LYS:HG3	1:A:486:ILE:HG23	1.89	0.55
1:A:456:THR:HG22	1:A:471:THR:OG1	2.07	0.55
1:A:81:ILE:HD12	1:A:147:ILE:HD12	1.87	0.55
1:A:118:ALA:HB2	1:A:467:VAL:HG21	1.87	0.55
1:B:14:ALA:O	1:B:18:GLN:HB2	2.07	0.55
1:A:72:LYS:HA	1:A:140:PRO:HD3	1.89	0.54
1:A:411:ILE:HD12	1:A:451:VAL:CG2	2.37	0.54
1:A:89:GLU:O	1:A:90:ASP:CB	2.55	0.54
1:B:71:ASN:O	1:B:488:GLU:CB	2.53	0.54
1:B:412:MET:HE2	1:B:451:VAL:HG12	1.90	0.54
1:A:118:ALA:HB1	1:A:467:VAL:HG21	1.89	0.54
1:A:318:ILE:HD12	1:A:322:GLN:CG	2.35	0.54
1:A:148:ASP:CB	1:A:154:THR:HG22	2.38	0.54
1:A:52:ARG:HD2	1:A:52:ARG:H	1.73	0.54
1:A:208:ARG:CD	1:A:308:GLU:HB3	2.38	0.54
1:B:196:ILE:HA	1:B:320:ASP:OD2	2.08	0.54
1:A:8:ILE:CD1	1:A:104:ILE:HG13	2.38	0.53
1:A:20:PHE:CD1	1:A:121:GLY:O	2.61	0.53
1:A:33:GLU:OE1	1:A:82:ASP:HB3	2.08	0.53
1:B:233:LYS:HD2	1:B:333:ASN:HB2	1.91	0.53
1:B:120:ASN:O	1:B:123:GLY:N	2.41	0.53
1:A:313:ALA:O	1:A:314:GLN:HB2	2.08	0.53
1:B:158:GLY:O	1:B:159:LEU:CB	2.56	0.53
1:A:72:LYS:HA	1:A:140:PRO:CD	2.39	0.53
1:A:183:GLY:HA2	1:A:403:TRP:CD2	2.44	0.53
1:A:292:LYS:HE2	1:A:302:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLN:HG2	1:B:237:ARG:HD3	1.91	0.53
1:A:428:ASN:C	1:A:428:ASN:HD22	2.12	0.53
1:B:54:ASP:CG	1:B:56:THR:HG22	2.29	0.53
1:B:347:GLU:HG2	1:B:372:ILE:HD13	1.90	0.53
1:B:217:GLY:O	1:B:228:ARG:NH1	2.42	0.53
1:B:471:THR:HA	1:B:474:LEU:HD22	1.90	0.53
1:A:191:ALA:O	1:A:394:ILE:HA	2.09	0.52
1:A:298:ILE:HG23	1:A:299:GLU:HG2	1.92	0.52
1:B:100:ILE:HD12	1:B:100:ILE:N	2.24	0.52
1:B:239:LEU:HD12	1:B:325:ILE:HD11	1.92	0.52
1:B:183:GLY:HA2	1:B:403:TRP:CG	2.45	0.52
1:B:418:MET:HG2	1:B:485:ALA:CB	2.39	0.52
1:A:167:ASP:OD2	1:A:167:ASP:N	2.42	0.52
1:B:226:THR:HB	1:B:228:ARG:CG	2.35	0.52
1:B:155:GLY:O	1:B:158:GLY:O	2.28	0.52
1:A:44:ALA:CB	1:A:51:VAL:HG21	2.39	0.52
1:A:58:ASN:HD22	1:A:159:LEU:HD13	1.73	0.52
1:A:326:ALA:HB1	1:B:389:LEU:HG	1.91	0.52
1:B:262:ILE:HA	1:B:351:ASN:HD21	1.75	0.52
1:A:83:MET:CE	1:A:117:GLY:HA3	2.40	0.52
1:A:209:GLN:HG3	1:A:269:THR:HG22	1.92	0.52
1:B:73:LYS:HD2	1:B:487:PRO:HG2	1.92	0.52
1:B:120:ASN:ND2	1:B:120:ASN:N	2.58	0.52
1:B:254:ARG:NH1	1:B:256:GLY:O	2.43	0.52
1:B:7:GLU:HG3	1:B:9:SER:H	1.75	0.52
1:B:413:ALA:HA	1:B:416:ARG:HG2	1.92	0.52
1:B:457:ILE:CG2	1:B:467:VAL:CG1	2.81	0.52
1:A:258:LEU:HD12	1:A:260:ASN:HB2	1.93	0.51
1:B:71:ASN:HB2	1:B:488:GLU:HG2	1.93	0.51
1:A:73:LYS:HG3	1:A:486:ILE:HG22	1.92	0.51
1:A:456:THR:CG2	1:A:471:THR:CG2	2.82	0.51
1:B:71:ASN:HB2	1:B:488:GLU:CB	2.36	0.51
1:B:440:LEU:O	1:B:443:GLU:HB3	2.11	0.51
1:A:100:ILE:HD12	1:A:100:ILE:N	2.24	0.51
1:B:198:ARG:NH1	1:B:251:VAL:O	2.32	0.51
1:B:432:ILE:HD11	1:B:436:LEU:HD11	1.92	0.51
1:B:120:ASN:C	1:B:122:ILE:N	2.63	0.51
1:A:432:ILE:HD11	1:A:436:LEU:HD11	1.93	0.51
1:A:40:ILE:HD12	1:A:128:LEU:HD21	1.93	0.51
1:A:120:ASN:C	1:A:122:ILE:H	2.15	0.51
1:B:443:GLU:OE1	1:B:444:PRO:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLN:HB2	1:A:115:THR:HG23	1.93	0.50
1:A:428:ASN:C	1:A:428:ASN:ND2	2.61	0.50
1:A:26:ILE:HD11	1:A:36:LEU:CD1	2.39	0.50
1:A:456:THR:HG23	1:A:468:LYS:HB3	1.93	0.50
1:A:205:PHE:CE2	1:A:273:PRO:HD3	2.46	0.50
1:B:167:ASP:O	1:B:168:ILE:HD13	2.12	0.50
1:B:420:GLU:OE2	1:B:420:GLU:O	2.28	0.50
1:A:193:THR:HG23	1:A:363:THR:HB	1.94	0.50
1:A:401:PRO:HG2	1:A:440:LEU:HA	1.94	0.50
1:B:75:VAL:CG2	1:B:141:ILE:CD1	2.90	0.50
1:A:456:THR:HG22	1:A:471:THR:CB	2.42	0.50
1:B:41:VAL:HG13	1:B:51:VAL:HG11	1.94	0.50
1:B:195:ASP:OD1	1:B:195:ASP:N	2.45	0.49
1:A:73:LYS:CG	1:A:486:ILE:HG22	2.42	0.49
1:A:394:ILE:HD12	1:A:396:PHE:CZ	2.47	0.49
1:B:410:GLU:O	1:B:414:ILE:HG12	2.12	0.49
1:B:80:HIS:HE1	1:B:82:ASP:O	1.93	0.49
1:B:305:PHE:HB3	1:B:307:GLU:HG3	1.93	0.49
1:A:8:ILE:HD13	1:A:104:ILE:CG1	2.43	0.49
1:A:200:ALA:HB2	1:A:314:GLN:HE22	1.77	0.49
1:B:285:ASN:CA	1:B:288:THR:HG22	2.39	0.49
1:A:60:PHE:HZ	1:A:159:LEU:HD11	1.76	0.49
1:A:119:ASP:HA	1:A:120:ASN:HA	1.54	0.49
1:B:8:ILE:H	1:B:8:ILE:CD1	2.25	0.49
1:A:88:ASN:HD22	1:A:89:GLU:H	1.61	0.49
1:B:54:ASP:OD2	1:B:56:THR:HG22	2.13	0.49
1:A:34:GLU:O	1:A:35:ALA:CB	2.60	0.48
1:A:124:MET:CE	1:A:145:LEU:HD22	2.43	0.48
1:A:208:ARG:HH11	1:A:277:GLN:HE21	1.60	0.48
1:B:174:SER:OG	1:B:453:PHE:HA	2.12	0.48
1:A:394:ILE:HD12	1:A:396:PHE:CE1	2.47	0.48
1:B:119:ASP:OD1	1:B:119:ASP:O	2.30	0.48
1:B:312:ASP:OD1	1:B:312:ASP:N	2.46	0.48
1:B:119:ASP:O	1:B:119:ASP:CG	2.52	0.48
1:B:72:LYS:HB3	1:B:486:ILE:HG21	1.95	0.48
1:B:292:LYS:O	1:B:296:GLY:HA3	2.14	0.48
1:A:382:MET:O	1:A:386:VAL:HG23	2.13	0.48
1:B:178:GLY:HA2	1:B:419:TYR:OH	2.14	0.48
1:A:51:VAL:CG2	1:A:61:ILE:HG12	2.34	0.48
1:A:207:THR:O	1:A:308:GLU:HB2	2.14	0.48
1:A:250:LEU:H	1:A:321:GLN:HE22	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:N	1:A:453:PHE:CD1	2.81	0.47
1:B:369:ARG:HG2	1:B:369:ARG:NH1	2.27	0.47
1:B:411:ILE:HG13	1:B:449:ASP:OD2	2.14	0.47
1:A:71:ASN:C	1:A:72:LYS:HG3	2.33	0.47
1:B:77:LEU:HD23	1:B:170:LEU:HB2	1.96	0.47
1:B:453:PHE:N	1:B:453:PHE:CD1	2.82	0.47
1:A:120:ASN:O	1:A:121:GLY:C	2.51	0.47
1:A:259:ARG:NH2	1:A:365:LEU:HG	2.28	0.47
1:B:108:TRP:HA	1:B:467:VAL:O	2.14	0.47
1:B:120:ASN:CB	1:B:123:GLY:HA3	2.42	0.47
1:A:188:ILE:HD12	1:A:396:PHE:CD2	2.50	0.47
1:B:459:PHE:N	1:B:460:PRO:HD3	2.30	0.47
1:B:206:ILE:CD1	1:B:207:THR:O	2.62	0.47
1:A:186:GLY:N	1:A:370:SER:O	2.43	0.47
1:B:23:ILE:CD1	1:B:36:LEU:HD21	2.45	0.47
1:B:248:LEU:HD12	1:B:248:LEU:C	2.35	0.47
1:B:454:GLY:HA2	1:B:475:PHE:CD2	2.50	0.47
1:B:486:ILE:CG1	1:B:487:PRO:HD2	2.36	0.47
1:A:138:HIS:CG	1:A:141:ILE:HD12	2.50	0.47
1:B:49:PHE:O	1:B:51:VAL:HG23	2.15	0.47
1:A:148:ASP:CG	1:A:154:THR:HG22	2.35	0.46
1:A:180:VAL:HG13	1:A:453:PHE:HB3	1.97	0.46
1:B:39:TYR:O	1:B:42:THR:HG22	2.15	0.46
1:B:72:LYS:HA	1:B:487:PRO:O	2.15	0.46
1:B:301:ASP:OD2	1:B:301:ASP:C	2.53	0.46
1:A:33:GLU:CG	1:A:147:ILE:HG13	2.46	0.46
1:B:171:ASN:HD22	1:B:438:CYS:HB3	1.80	0.46
1:A:376:ARG:O	1:A:380:GLU:HG3	2.15	0.46
1:B:438:CYS:HA	1:B:441:PHE:CE1	2.50	0.46
1:A:112:LYS:HE3	1:A:113:GLY:H	1.80	0.46
1:A:206:ILE:HD13	1:A:277:GLN:HE22	1.81	0.46
1:B:224:ILE:HD12	1:B:262:ILE:HD11	1.97	0.46
1:B:372:ILE:N	1:B:372:ILE:HD12	2.30	0.46
1:A:88:ASN:CB	1:A:113:GLY:HA2	2.41	0.46
1:A:312:ASP:CA	1:A:313:ALA:HB3	2.41	0.46
1:B:359:GLU:CD	1:B:359:GLU:N	2.60	0.46
1:B:301:ASP:OD2	1:B:302:ILE:N	2.48	0.46
1:A:83:MET:CG	1:A:84:VAL:N	2.78	0.46
1:A:117:GLY:C	1:A:119:ASP:N	2.70	0.46
1:B:159:LEU:HA	1:B:159:LEU:HD23	1.68	0.46
1:A:9:SER:HB3	1:A:18:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD23	1:A:159:LEU:O	2.15	0.46
1:B:174:SER:HB2	1:B:181:TYR:HE1	1.81	0.46
1:B:230:ASN:ND2	1:B:232:ASN:HB2	2.26	0.46
1:A:83:MET:HG2	1:A:84:VAL:H	1.81	0.45
1:B:71:ASN:O	1:B:72:LYS:C	2.55	0.45
1:B:230:ASN:ND2	1:B:233:LYS:H	2.13	0.45
1:B:420:GLU:O	1:B:420:GLU:CG	2.63	0.45
1:B:462:SER:C	1:B:464:ASP:H	2.19	0.45
1:A:83:MET:HE2	1:A:117:GLY:HA3	1.98	0.45
1:A:177:GLU:HG2	1:A:474:LEU:HD23	1.98	0.45
1:A:54:ASP:HB2	1:A:55:PRO:HD2	1.99	0.45
1:A:208:ARG:HD3	1:A:277:GLN:NE2	2.30	0.45
1:A:324:PHE:CD2	1:A:325:ILE:HD12	2.51	0.45
1:A:372:ILE:CG2	1:A:374:SER:HB3	2.46	0.45
1:B:58:ASN:HA	1:B:147:ILE:CD1	2.47	0.45
1:A:122:ILE:CG2	1:A:455:PRO:CG	2.64	0.45
1:A:332:PRO:HG3	1:A:382:MET:HE2	1.97	0.45
1:A:369:ARG:HG2	1:A:369:ARG:HH11	1.82	0.45
1:A:455:PRO:CG	1:A:457:ILE:HD11	2.40	0.45
1:A:489:LYS:HD2	1:A:489:LYS:HA	1.68	0.45
1:B:84:VAL:HA	1:B:85:PRO:HD3	1.73	0.45
1:B:75:VAL:CG2	1:B:141:ILE:HD13	2.40	0.45
1:A:474:LEU:O	1:A:475:PHE:C	2.55	0.45
1:B:86:GLN:HG3	1:B:461:HIS:O	2.17	0.45
1:B:221:GLY:O	1:B:433:HIS:HB3	2.16	0.45
1:B:279:LYS:O	1:B:282:GLU:HB2	2.17	0.45
1:A:479:MET:HE1	1:A:483:LEU:HG	1.98	0.45
1:B:257:SER:HG	1:B:258:LEU:HG	1.82	0.45
1:A:418:MET:O	1:A:422:ILE:HG12	2.17	0.44
1:B:284:PHE:O	1:B:288:THR:HG22	2.16	0.44
1:A:315:VAL:HG12	1:A:316:PHE:O	2.17	0.44
1:B:57:GLY:O	1:B:147:ILE:HD11	2.17	0.44
1:B:119:ASP:HA	1:B:120:ASN:HA	1.52	0.44
1:B:120:ASN:O	1:B:121:GLY:C	2.56	0.44
1:A:171:ASN:O	1:A:452:SER:HA	2.17	0.44
1:A:464:ASP:O	1:A:466:LYS:N	2.51	0.44
1:B:213:LYS:HG2	1:B:214:GLY:N	2.32	0.44
1:B:488:GLU:O	1:B:488:GLU:OE1	2.34	0.44
1:A:74:GLY:H	1:A:140:PRO:HG2	1.82	0.44
1:B:86:GLN:HB2	1:B:115:THR:HG23	1.98	0.44
1:A:157:PHE:O	1:A:157:PHE:CD2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:HA	1:A:288:THR:CG2	2.48	0.44
1:B:425:HIS:O	1:B:426:LYS:HB2	2.16	0.44
1:A:120:ASN:ND2	1:A:120:ASN:N	2.63	0.44
1:A:188:ILE:HD13	1:A:189:ASP:C	2.36	0.44
1:A:258:LEU:HD12	1:A:260:ASN:CB	2.48	0.44
1:A:100:ILE:O	1:A:102:PRO:HD3	2.17	0.44
1:A:157:PHE:O	1:A:157:PHE:CG	2.69	0.44
1:A:70:GLU:C	1:A:72:LYS:H	2.21	0.44
1:A:73:LYS:HD2	1:A:73:LYS:HA	1.43	0.44
1:A:88:ASN:HB2	1:A:113:GLY:CA	2.44	0.44
1:A:60:PHE:HZ	1:A:159:LEU:CD1	2.31	0.43
1:A:119:ASP:O	1:A:119:ASP:CG	2.56	0.43
1:A:250:LEU:H	1:A:321:GLN:NE2	2.16	0.43
1:A:60:PHE:CD1	1:A:60:PHE:N	2.86	0.43
1:A:84:VAL:CG2	1:A:150:GLU:HG2	2.46	0.43
1:B:66:THR:CG2	1:B:138:HIS:CE1	3.01	0.43
1:A:137:LYS:O	1:A:484:GLU:HG2	2.18	0.43
1:B:54:ASP:OD1	1:B:56:THR:HG22	2.19	0.43
1:A:69:MET:HE2	1:A:69:MET:N	2.34	0.43
1:B:201:ILE:H	1:B:201:ILE:HG13	1.35	0.43
1:B:65:ALA:HB1	1:B:69:MET:O	2.18	0.43
1:B:248:LEU:HD12	1:B:248:LEU:O	2.17	0.43
1:A:28:HIS:CE1	1:A:83:MET:CE	2.99	0.43
1:A:69:MET:HE3	1:A:69:MET:HB2	1.90	0.43
1:B:38:GLN:O	1:B:39:TYR:C	2.56	0.43
1:B:51:VAL:HG22	1:B:61:ILE:HG12	2.01	0.43
1:B:268:VAL:O	1:B:268:VAL:HG13	2.19	0.43
1:A:119:ASP:OD1	1:A:119:ASP:O	2.35	0.43
1:B:156:ALA:HB3	1:B:440:LEU:CD2	2.48	0.43
1:B:174:SER:HB2	1:B:181:TYR:CE1	2.54	0.43
1:A:201:ILE:HD12	1:A:315:VAL:HG23	2.00	0.43
1:B:85:PRO:HA	1:B:95:PHE:CE2	2.54	0.43
1:B:272:LEU:HD11	1:B:277:GLN:HA	2.01	0.43
1:B:443:GLU:HB3	1:B:444:PRO:CD	2.48	0.43
1:A:45:THR:O	1:A:48:GLY:N	2.33	0.43
1:A:171:ASN:ND2	1:A:173:ASP:N	2.60	0.43
1:A:226:THR:HG22	1:A:227:GLY:H	1.84	0.43
1:B:318:ILE:HG23	1:B:319:ALA:H	1.84	0.43
1:A:159:LEU:CD2	1:A:159:LEU:C	2.87	0.42
1:A:215:LEU:O	1:A:264:ARG:HB2	2.18	0.42
1:A:263:PRO:HD3	1:A:351:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HA	1:B:488:GLU:HB3	2.00	0.42
1:B:359:GLU:O	1:B:360:ASN:CB	2.67	0.42
1:A:140:PRO:O	1:A:141:ILE:HG13	2.20	0.42
1:B:83:MET:HG2	1:B:84:VAL:H	1.84	0.42
1:B:156:ALA:HB2	1:B:437:GLU:HG3	2.02	0.42
1:A:150:GLU:O	1:A:150:GLU:CG	2.67	0.42
1:A:202:PRO:HG2	1:A:205:PHE:CE1	2.54	0.42
1:A:249:ARG:HB3	1:A:315:VAL:CG1	2.39	0.42
1:B:250:LEU:N	1:B:321:GLN:NE2	2.62	0.42
1:A:56:THR:HG21	1:A:158:GLY:HA3	2.01	0.42
1:A:141:ILE:HD11	1:A:483:LEU:HD22	2.01	0.42
1:A:201:ILE:HD11	1:A:314:GLN:H	1.84	0.42
1:A:377:SER:O	1:A:378:GLN:C	2.57	0.42
1:B:71:ASN:HD22	1:B:71:ASN:N	2.01	0.42
1:B:290:LEU:O	1:B:293:THR:HB	2.20	0.42
1:B:124:MET:HE3	1:B:145:LEU:HD22	2.00	0.42
1:A:77:LEU:HB2	1:A:143:VAL:HG22	2.02	0.42
1:A:122:ILE:HG21	1:A:455:PRO:CB	2.46	0.42
1:B:71:ASN:HB2	1:B:488:GLU:CG	2.50	0.42
1:A:57:GLY:O	1:A:147:ILE:HD13	2.19	0.42
1:A:372:ILE:HD13	1:A:404:LYS:HB2	2.01	0.42
1:B:28:HIS:ND1	1:B:28:HIS:N	2.68	0.42
1:B:230:ASN:HD22	1:B:230:ASN:C	2.23	0.42
1:A:85:PRO:O	1:A:86:GLN:HG2	2.20	0.41
1:B:41:VAL:HG13	1:B:51:VAL:CG1	2.49	0.41
1:B:108:TRP:CD2	1:B:466:LYS:HD3	2.54	0.41
1:B:462:SER:O	1:B:464:ASP:N	2.53	0.41
1:A:482:LEU:O	1:A:485:ALA:N	2.51	0.41
1:A:37:ALA:O	1:A:41:VAL:HG22	2.21	0.41
1:A:312:ASP:HB2	1:A:313:ALA:HB3	2.02	0.41
1:B:359:GLU:O	1:B:360:ASN:HB2	2.20	0.41
1:A:26:ILE:O	1:A:26:ILE:CG1	2.67	0.41
1:A:88:ASN:HD22	1:A:89:GLU:N	2.18	0.41
1:A:471:THR:HA	1:A:474:LEU:HD22	2.02	0.41
1:B:438:CYS:HB2	1:B:450:MET:CE	2.49	0.41
1:B:457:ILE:CB	1:B:467:VAL:HG12	2.45	0.41
1:A:188:ILE:HD13	1:A:188:ILE:C	2.41	0.41
1:B:136:ILE:HG23	1:B:480:VAL:HG13	2.03	0.41
1:B:85:PRO:O	1:B:86:GLN:HG2	2.20	0.41
1:A:84:VAL:HG21	1:A:461:HIS:CD2	2.56	0.41
1:A:148:ASP:OD2	1:A:154:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ALA:HB2	1:A:437:GLU:HG3	2.02	0.41
1:B:72:LYS:HB2	1:B:139:GLY:CA	2.51	0.41
1:B:126:SER:O	1:B:130:VAL:HG23	2.20	0.41
1:A:198:ARG:NH2	1:A:359:GLU:HA	2.35	0.41
1:A:235:ILE:O	1:A:239:LEU:HG	2.20	0.41
1:A:462:SER:C	1:A:464:ASP:H	2.24	0.41
1:B:196:ILE:HG22	1:B:320:ASP:CB	2.51	0.41
1:B:318:ILE:O	1:B:322:GLN:HG3	2.20	0.41
1:B:355:ILE:N	1:B:355:ILE:CD1	2.84	0.41
1:B:72:LYS:CB	1:B:139:GLY:HA3	2.51	0.41
1:A:208:ARG:HD2	1:A:308:GLU:HB3	2.03	0.40
1:B:117:GLY:C	1:B:119:ASP:N	2.74	0.40
1:B:235:ILE:O	1:B:236:GLY:C	2.60	0.40
1:A:75:VAL:HG12	1:A:76:VAL:N	2.36	0.40
1:A:479:MET:O	1:A:479:MET:HE2	2.21	0.40
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.93	0.40
1:B:16:LEU:HD21	1:B:122:ILE:HG22	2.00	0.40
1:B:76:VAL:HA	1:B:142:GLU:O	2.22	0.40
1:B:120:ASN:O	1:B:122:ILE:N	2.54	0.40
1:B:254:ARG:NH2	1:B:356:THR:CG2	2.53	0.40
1:A:176:GLN:HE21	1:A:176:GLN:HB2	1.68	0.40
1:B:60:PHE:HZ	1:B:159:LEU:HD21	1.86	0.40
1:B:136:ILE:HG22	1:B:137:LYS:O	2.22	0.40
1:B:343:GLU:H	1:B:343:GLU:CD	2.24	0.40
1:B:411:ILE:HD13	1:B:451:VAL:HG13	2.04	0.40
1:A:118:ALA:CB	1:A:467:VAL:CG2	2.92	0.40
1:A:163:TRP:O	1:A:164:LEU:HD23	2.20	0.40
1:A:454:GLY:HA2	1:A:475:PHE:CE2	2.56	0.40
1:A:482:LEU:HA	1:A:485:ALA:HB3	2.02	0.40
1:B:253:PHE:HD2	1:B:254:ARG:N	2.20	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	488/490 (100%)	448 (92%)	32 (7%)	8 (2%)	9	40
1	B	488/490 (100%)	444 (91%)	39 (8%)	5 (1%)	15	53
All	All	976/980 (100%)	892 (91%)	71 (7%)	13 (1%)	12	45

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	74	GLY
1	A	90	ASP
1	A	313	ALA
1	B	159	LEU
1	A	35	ALA
1	A	121	GLY
1	A	465	GLU
1	B	423	TYR
1	B	487	PRO
1	B	459	PHE
1	B	101	GLN
1	A	459	PHE

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	402/402 (100%)	341 (85%)	61 (15%)	3	14
1	B	402/402 (100%)	334 (83%)	68 (17%)	2	11
All	All	804/804 (100%)	675 (84%)	129 (16%)	2	12

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	16	LEU
1	A	26	ILE
1	A	33	GLU
1	A	52	ARG
1	A	53	ARG
1	A	56	THR
1	A	69	MET
1	A	73	LYS
1	A	78	GLN
1	A	87	LYS
1	A	88	ASN
1	A	89	GLU
1	A	107	GLU
1	A	112	LYS
1	A	119	ASP
1	A	128	LEU
1	A	144	LEU
1	A	159	LEU
1	A	160	GLU
1	A	167	ASP
1	A	169	LEU
1	A	177	GLU
1	A	180	VAL
1	A	188	ILE
1	A	193	THR
1	A	201	ILE
1	A	211	THR
1	A	226	THR
1	A	230	ASN
1	A	245	GLU
1	A	251	VAL
1	A	253	PHE
1	A	258	LEU
1	A	259	ARG
1	A	260	ASN
1	A	276	ASN
1	A	288	THR
1	A	289	GLU
1	A	297	LYS
1	A	308	GLU
1	A	312	ASP
1	A	318	ILE

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Mol	Chain	Res	Type
1	A	350	LEU
1	A	351	ASN
1	A	363	THR
1	A	378	GLN
1	A	388	GLU
1	A	408	ASP
1	A	411	ILE
1	A	428	ASN
1	A	443	GLU
1	A	452	SER
1	A	462	SER
1	A	466	LYS
1	A	470	ASP
1	A	471	THR
1	A	474	LEU
1	A	478	GLN
1	A	479	MET
1	A	489	LYS
1	B	2	SER
1	B	9	SER
1	B	18	GLN
1	B	30	SER
1	B	42	THR
1	B	50	ASP
1	B	52	ARG
1	B	69	MET
1	B	71	ASN
1	B	89	GLU
1	B	90	ASP
1	B	112	LYS
1	B	115	THR
1	B	119	ASP
1	B	120	ASN
1	B	122	ILE
1	B	147	ILE
1	B	154	THR
1	B	160	GLU
1	B	168	ILE
1	B	169	LEU
1	B	175	GLU
1	B	193	THR
1	B	195	ASP

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Mol	Chain	Res	Type
1	B	197	THR
1	B	201	ILE
1	B	206	ILE
1	B	211	THR
1	B	226	THR
1	B	230	ASN
1	B	246	LEU
1	B	247	ASP
1	B	251	VAL
1	B	253	PHE
1	B	254	ARG
1	B	257	SER
1	B	258	LEU
1	B	280	LEU
1	B	282	GLU
1	B	297	LYS
1	B	308	GLU
1	B	312	ASP
1	B	315	VAL
1	B	323	ARG
1	B	348	THR
1	B	350	LEU
1	B	359	GLU
1	B	363	THR
1	B	374	SER
1	B	388	GLU
1	B	406	ASP
1	B	412	MET
1	B	418	MET
1	B	420	GLU
1	B	425	HIS
1	B	428	ASN
1	B	430	MET
1	B	440	LEU
1	B	443	GLU
1	B	447	ASN
1	B	453	PHE
1	B	464	ASP
1	B	467	VAL
1	B	471	THR
1	B	474	LEU
1	B	486	ILE

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Mol	Chain	Res	Type
1	B	488	GLU
1	B	489	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	78	GLN
1	A	88	ASN
1	A	138	HIS
1	A	171	ASN
1	A	230	ASN
1	A	260	ASN
1	A	277	GLN
1	A	314	GLN
1	A	321	GLN
1	A	329	ASN
1	A	351	ASN
1	A	384	GLN
1	A	428	ASN
1	A	473	GLN
1	B	71	ASN
1	B	78	GLN
1	B	86	GLN
1	B	97	GLN
1	B	120	ASN
1	B	138	HIS
1	B	176	GLN
1	B	230	ASN
1	B	321	GLN
1	B	351	ASN
1	B	428	ASN
1	B	461	HIS

5.3.3 RNA (i)

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 4 ligands modelled in this entry, 4 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, 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	490/490 (100%)	-0.42	2 (0%)	92	79	43, 81, 130, 203	0
1	B	490/490 (100%)	-0.40	5 (1%)	82	59	41, 81, 139, 249	0
All	All	980/980 (100%)	-0.41	7 (0%)	87	69	41, 81, 135, 249	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	ALA	3.5
1	A	178	GLY	3.2
1	A	490	ALA	3.2
1	B	425	HIS	3.1
1	B	421	GLY	3.0
1	B	424	GLY	2.5
1	B	311	THR	2.5

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, 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	492	1/1	0.36	0.12	105,105,105,105	0
2	ZN	A	491	1/1	0.90	0.22	121,121,121,121	0
2	ZN	B	491	1/1	0.93	0.28	110,110,110,110	0
2	ZN	B	492	1/1	0.98	0.08	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.