



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:20 AM UTC

PDB ID : 6KXG / pdb_00006kxg
Title : Crystal structure of caspase-11-CARD
Authors : Liu, M.Z.Y.; Jin, T.C.
Deposited on : 2019-09-11
Resolution : 2.81 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

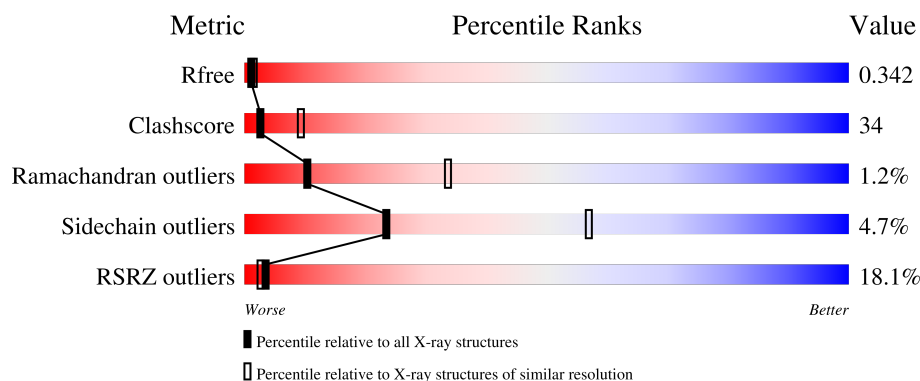
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	462	13% 55% 35% 8%
1	B	462	19% 46% 36% 14%
1	C	462	17% 50% 39% 9%
1	D	462	16% 48% 37% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12882 atoms, of which 0 are hydrogens and 0 are deuteriums.

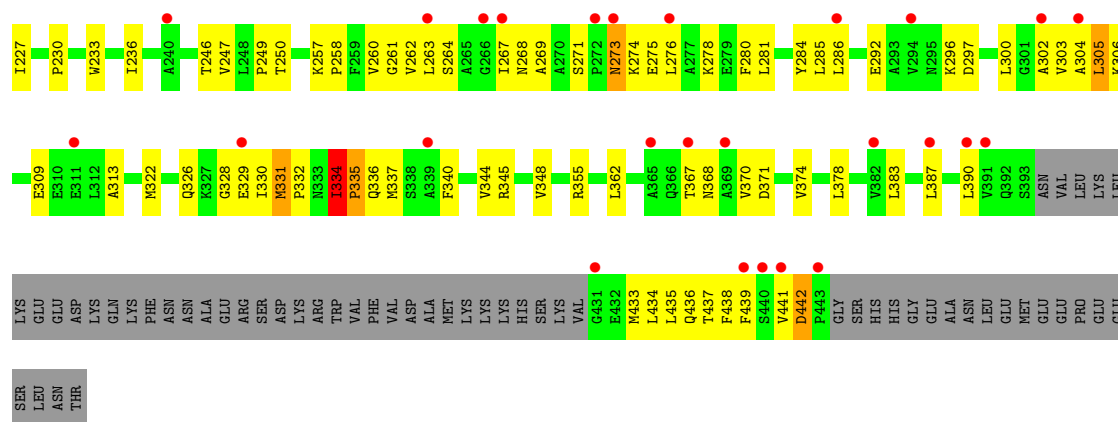
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called caspase-11-CARD.

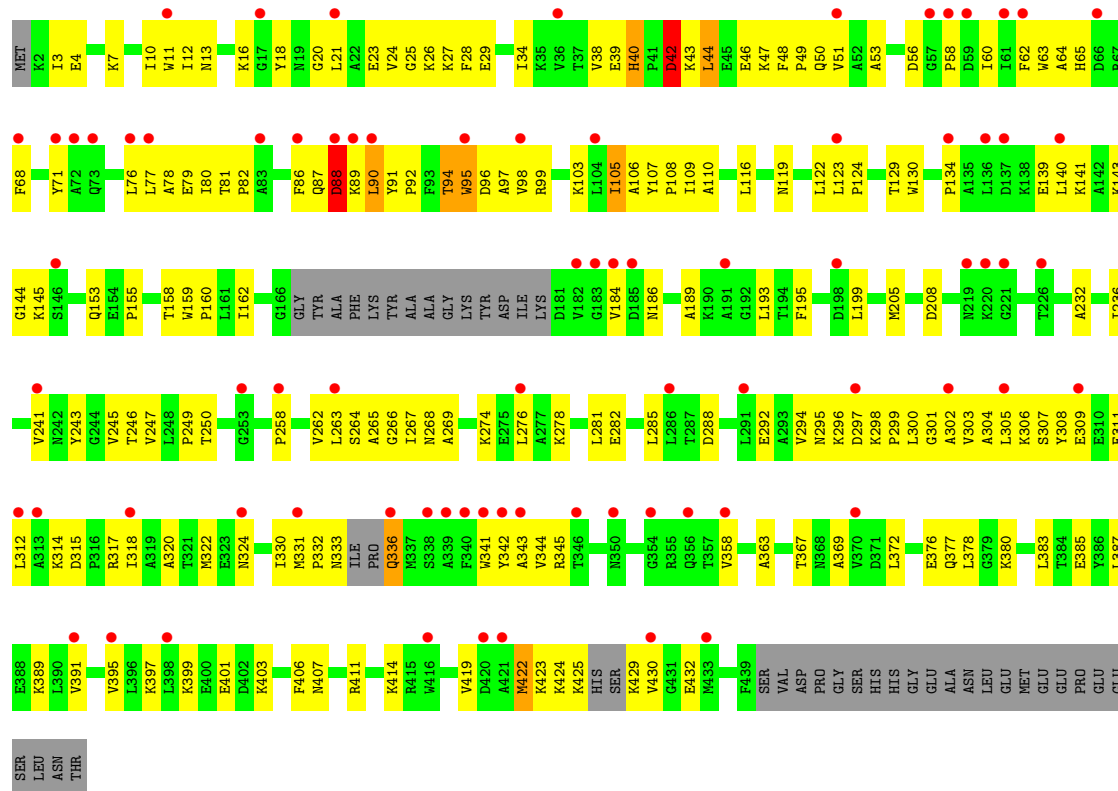
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3319	2140	541	630	8			
1	B	399	Total	C	N	O	S	0	0	0
			3079	1987	495	590	7			
1	C	419	Total	C	N	O	S	0	0	0
			3258	2096	534	620	8			
1	D	415	Total	C	N	O	S	0	0	0
			3223	2074	525	616	8			

- Molecule 2 is water.

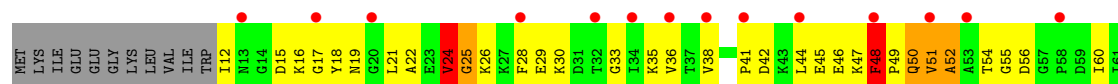
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		

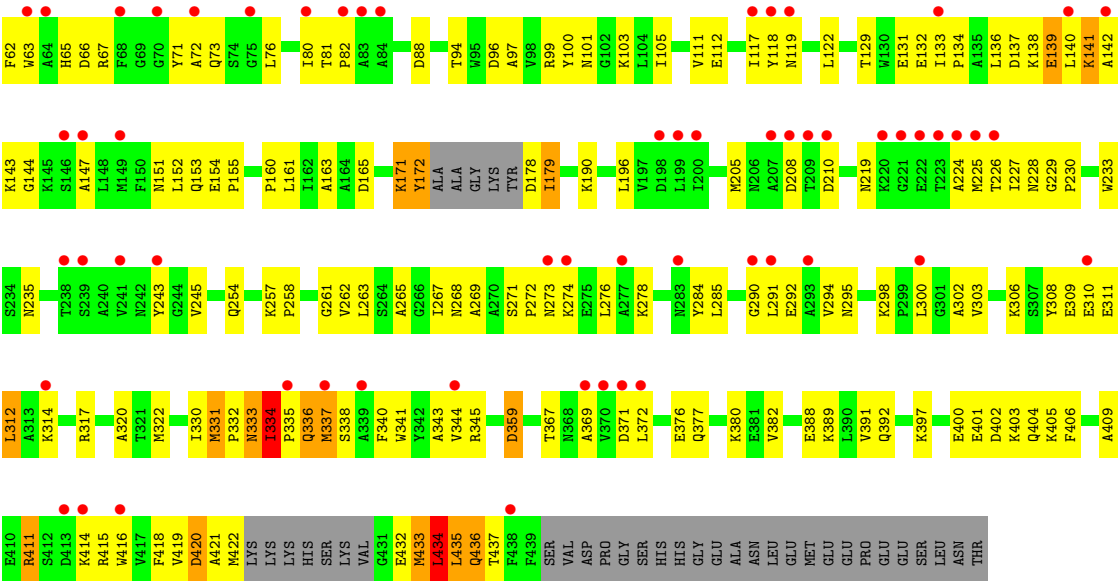


• Molecule 1: caspase-11-CARD



• Molecule 1: caspase-11-CARD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.31Å 145.16Å 187.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.67 – 2.81 38.67 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.67-2.81) 97.3 (38.67-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.305 , 0.340 0.307 , 0.342	Depositor DCC
R_{free} test set	2573 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 92.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12882	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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

5.1 Standard geometry

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	0.36	0/3394	0.59	5/4603 (0.1%)
1	B	0.35	1/3149 (0.0%)	0.65	8/4278 (0.2%)
1	C	0.32	0/3326	0.57	4/4504 (0.1%)
1	D	0.36	0/3294	0.66	6/4467 (0.1%)
All	All	0.35	1/13163 (0.0%)	0.62	23/17852 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	ILE	CA-CB	-5.64	1.51	1.55

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	ALA	N-CA-C	-9.35	102.00	113.97
1	B	331	MET	CA-C-N	7.67	127.72	119.89
1	B	331	MET	C-N-CA	7.67	127.72	119.89
1	C	18	TYR	N-CA-C	-7.45	104.34	113.50
1	D	312	LEU	N-CA-C	-6.85	104.74	113.23
1	B	62	PHE	N-CA-C	6.68	119.79	108.90
1	B	61	ILE	N-CA-C	6.43	115.55	107.70
1	D	25	GLY	N-CA-C	-6.33	105.88	113.99
1	C	40	HIS	CA-C-N	6.24	127.64	119.84
1	C	40	HIS	C-N-CA	6.24	127.64	119.84
1	A	401	GLU	N-CA-C	-5.93	107.27	114.75
1	A	265	ALA	N-CA-C	5.62	118.23	109.52
1	D	420	ASP	N-CA-C	-5.57	105.11	111.07
1	B	190	LYS	CB-CA-C	5.55	119.50	110.96
1	D	24	VAL	CB-CA-C	-5.53	106.20	111.06
1	B	334	ILE	N-CA-C	-5.52	102.69	108.15
1	B	191	ALA	N-CA-C	5.52	118.00	111.33
1	A	434	LEU	CA-C-N	-5.17	117.60	123.13
1	A	434	LEU	C-N-CA	-5.17	117.60	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	TRP	CB-CA-C	-5.16	100.67	109.03
1	A	125	ASN	CA-CB-CG	5.16	117.75	112.60
1	B	190	LYS	N-CA-C	-5.07	105.45	110.97
1	D	24	VAL	N-CA-C	-5.02	107.94	112.96

There are no chirality outliers.

There are no planarity outliers.

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	3319	0	3306	178	0
1	B	3079	0	3055	260	0
1	C	3258	0	3257	228	0
1	D	3223	0	3198	222	0
2	A	3	0	0	0	0
All	All	12882	0	12816	871	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 34.

All (871) 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:12:ILE:HD11	1:B:62:PHE:CD2	1.41	1.51
1:B:66:ASP:HB3	1:B:331:MET:SD	1.66	1.34
1:C:63:TRP:CD1	1:C:64:ALA:H	1.44	1.33
1:B:80:ILE:HD12	1:B:107:TYR:CZ	1.67	1.28
1:C:63:TRP:CD1	1:C:64:ALA:N	2.01	1.26
1:B:11:TRP:CB	1:B:61:ILE:HD11	1.65	1.26
1:B:11:TRP:CH2	1:B:58:PRO:HD3	1.70	1.25
1:D:24:VAL:CG2	1:D:28:PHE:HD2	1.51	1.23
1:D:334:ILE:HG22	1:D:335:PRO:CD	1.70	1.21
1:C:106:ALA:HB1	1:C:265:ALA:O	1.38	1.21
1:D:24:VAL:HG21	1:D:28:PHE:CD2	1.77	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:O	1:C:49:PRO:HD2	1.42	1.18
1:B:12:ILE:CD1	1:B:62:PHE:CD2	2.30	1.14
1:C:91:TYR:HB2	1:C:94:THR:HG22	1.27	1.14
1:D:334:ILE:CG2	1:D:335:PRO:HD3	1.76	1.14
1:B:79:GLU:CD	1:B:103:LYS:HB3	1.71	1.14
1:D:48:PHE:N	1:D:49:PRO:HD3	1.63	1.14
1:C:305:LEU:HD21	1:C:307:SER:OG	1.47	1.13
1:B:11:TRP:HB2	1:B:61:ILE:HD11	1.12	1.12
1:D:24:VAL:HG22	1:D:29:GLU:HG3	1.16	1.11
1:B:8:LEU:HD22	1:B:273:ASN:HD22	1.13	1.11
1:D:334:ILE:CG2	1:D:335:PRO:CD	2.29	1.11
1:B:11:TRP:CA	1:B:61:ILE:HD11	1.80	1.10
1:A:107:TYR:OH	1:A:278:LYS:HE2	1.51	1.10
1:B:8:LEU:HD21	1:B:273:ASN:HB2	1.29	1.09
1:D:334:ILE:HB	1:D:335:PRO:HD2	1.33	1.08
1:B:11:TRP:HB2	1:B:61:ILE:CD1	1.85	1.07
1:B:45:GLU:HG3	1:B:67:ARG:NH1	1.68	1.07
1:B:98:VAL:HG12	1:B:105:ILE:CG1	1.85	1.06
1:B:80:ILE:CD1	1:B:107:TYR:CZ	2.38	1.06
1:D:48:PHE:H	1:D:49:PRO:HD3	1.14	1.06
1:B:11:TRP:H	1:B:61:ILE:CD1	1.67	1.06
1:B:98:VAL:O	1:B:105:ILE:HG12	1.56	1.06
1:C:91:TYR:CD1	1:C:306:LYS:HE2	1.90	1.06
1:B:8:LEU:HD11	1:B:59:ASP:HB2	1.32	1.05
1:B:98:VAL:CG1	1:B:105:ILE:HG13	1.84	1.05
1:D:52:ALA:HB2	1:D:268:ASN:HD21	1.20	1.05
1:A:8:LEU:HB3	1:A:36:VAL:CG1	1.87	1.05
1:B:12:ILE:CD1	1:B:62:PHE:HD2	1.69	1.05
1:A:60:ILE:HD11	1:A:277:ALA:HB1	1.06	1.04
1:D:308:TYR:O	1:D:312:LEU:HD12	1.55	1.04
1:D:334:ILE:CB	1:D:335:PRO:CD	2.35	1.04
1:D:48:PHE:N	1:D:49:PRO:CD	2.21	1.04
1:A:8:LEU:CB	1:A:36:VAL:HG12	1.88	1.04
1:D:24:VAL:CG2	1:D:28:PHE:CD2	2.38	1.03
1:B:98:VAL:HG12	1:B:105:ILE:HG13	1.04	1.03
1:D:24:VAL:HG21	1:D:28:PHE:HD2	0.85	1.02
1:A:5:GLU:HB3	1:A:272:PRO:HB2	1.39	1.01
1:B:60:ILE:HG22	1:B:267:ILE:HG23	1.40	1.01
1:A:284:TYR:O	1:A:287:THR:HG23	1.61	1.01
1:C:91:TYR:HA	1:C:306:LYS:HE3	1.41	1.01
1:B:8:LEU:HD21	1:B:273:ASN:CB	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:CD2	1:B:273:ASN:HD22	1.73	1.00
1:C:91:TYR:HA	1:C:306:LYS:CE	1.92	1.00
1:B:63:TRP:HA	1:B:63:TRP:CE3	1.94	1.00
1:B:65:HIS:CE1	1:B:331:MET:HB3	1.95	1.00
1:A:8:LEU:HB3	1:A:36:VAL:HG12	1.03	0.99
1:C:48:PHE:HZ	1:C:77:LEU:HD11	1.26	0.99
1:C:87:GLN:O	1:C:88:ASP:HB2	1.58	0.99
1:D:24:VAL:HG23	1:D:28:PHE:HB3	1.39	0.99
1:B:219:ASN:OD1	1:B:236:ILE:HG22	1.62	0.99
1:D:334:ILE:CB	1:D:335:PRO:HD2	1.93	0.99
1:D:52:ALA:CB	1:D:268:ASN:HD21	1.77	0.97
1:A:81:THR:N	1:A:278:LYS:HZ1	1.63	0.97
1:A:5:GLU:HB2	1:A:273:ASN:ND2	1.79	0.96
1:B:8:LEU:CD1	1:B:59:ASP:HB2	1.95	0.96
1:A:268:ASN:HB3	1:A:271:SER:HB2	1.47	0.96
1:A:5:GLU:HB2	1:A:273:ASN:HD21	1.27	0.95
1:A:60:ILE:HD11	1:A:277:ALA:CB	1.96	0.95
1:B:12:ILE:HD11	1:B:62:PHE:CG	2.01	0.94
1:B:66:ASP:CB	1:B:331:MET:SD	2.56	0.94
1:A:81:THR:H	1:A:278:LYS:HZ1	0.96	0.94
1:C:91:TYR:CA	1:C:306:LYS:HE3	1.97	0.93
1:B:79:GLU:CD	1:B:103:LYS:CB	2.42	0.93
1:D:334:ILE:HB	1:D:335:PRO:CD	1.94	0.92
1:C:63:TRP:HD1	1:C:64:ALA:N	1.53	0.91
1:A:81:THR:H	1:A:278:LYS:NZ	1.69	0.91
1:B:12:ILE:HD11	1:B:62:PHE:HD2	1.11	0.91
1:D:137:ASP:OD1	1:D:141:LYS:HG2	1.70	0.91
1:B:11:TRP:N	1:B:61:ILE:CD1	2.34	0.91
1:C:98:VAL:HG13	1:C:105:ILE:HG23	1.54	0.90
1:D:21:LEU:HD23	1:D:38:VAL:HG11	1.54	0.90
1:D:24:VAL:CG2	1:D:29:GLU:HG3	2.02	0.89
1:D:179:ILE:HB	1:D:334:ILE:HD11	1.53	0.89
1:B:79:GLU:OE1	1:B:103:LYS:HG2	1.72	0.89
1:D:171:LYS:HG3	1:D:330:ILE:HG12	1.52	0.88
1:D:334:ILE:HG22	1:D:335:PRO:HD3	0.92	0.88
1:D:308:TYR:O	1:D:312:LEU:CD1	2.22	0.88
1:B:8:LEU:HD11	1:B:59:ASP:CB	2.03	0.87
1:B:80:ILE:HD13	1:B:107:TYR:CE2	2.08	0.87
1:C:46:GLU:O	1:C:49:PRO:CD	2.23	0.87
1:D:52:ALA:HB2	1:D:268:ASN:ND2	1.90	0.87
1:D:139:GLU:OE2	1:D:139:GLU:N	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:HB2	1:C:94:THR:CG2	2.03	0.87
1:C:65:HIS:HE1	1:C:330:ILE:HG23	1.39	0.87
1:D:24:VAL:HG23	1:D:28:PHE:CB	2.04	0.86
1:B:110:ALA:HB3	1:B:263:LEU:HD21	1.57	0.86
1:D:309:GLU:HA	1:D:312:LEU:HD13	1.55	0.86
1:B:11:TRP:CZ3	1:B:58:PRO:HD3	2.09	0.86
1:C:91:TYR:OH	1:C:309:GLU:HG2	1.75	0.86
1:D:401:GLU:HA	1:D:404:GLN:OE1	1.76	0.85
1:B:11:TRP:HZ3	1:B:51:VAL:HG11	1.42	0.85
1:B:9:VAL:C	1:B:10:ILE:HG13	1.99	0.85
1:B:63:TRP:HA	1:B:63:TRP:HE3	1.32	0.85
1:B:99:ARG:HB2	1:B:99:ARG:CZ	2.05	0.84
1:B:8:LEU:HD22	1:B:273:ASN:ND2	1.93	0.84
1:D:228:ASN:HD22	1:D:229:GLY:H	1.23	0.84
1:D:404:GLN:OE1	1:D:404:GLN:N	2.11	0.83
1:B:79:GLU:OE2	1:B:103:LYS:HB3	1.78	0.83
1:D:334:ILE:CG2	1:D:335:PRO:HD2	2.03	0.83
1:A:81:THR:N	1:A:278:LYS:NZ	2.26	0.83
1:D:331:MET:HG3	1:D:332:PRO:HD2	1.61	0.83
1:B:11:TRP:CZ3	1:B:51:VAL:HG11	2.14	0.82
1:D:24:VAL:HG22	1:D:29:GLU:CG	2.06	0.82
1:A:107:TYR:OH	1:A:278:LYS:CE	2.27	0.82
1:A:399:LYS:HA	1:A:403:LYS:HB2	1.58	0.82
1:B:26:LYS:HZ2	1:B:30:LYS:HD3	1.44	0.82
1:C:92:PRO:HD3	1:C:306:LYS:NZ	1.94	0.82
1:B:80:ILE:CD1	1:B:107:TYR:CE2	2.62	0.81
1:A:413:ASP:OD1	1:A:416:TRP:HB2	1.80	0.81
1:B:103:LYS:H	1:B:103:LYS:HD2	1.46	0.80
1:C:21:LEU:HD23	1:C:38:VAL:HG23	1.63	0.80
1:C:90:LEU:HB2	1:C:95:TRP:CZ2	2.17	0.80
1:B:11:TRP:H	1:B:61:ILE:HD13	1.46	0.80
1:B:286:LEU:O	1:B:305:LEU:HD11	1.80	0.80
1:C:106:ALA:HB2	1:C:266:GLY:HA2	1.62	0.80
1:B:45:GLU:HG3	1:B:67:ARG:HH11	1.46	0.80
1:B:65:HIS:CE1	1:B:260:VAL:O	2.35	0.80
1:C:48:PHE:CZ	1:C:77:LEU:HD11	2.14	0.80
1:D:434:LEU:H	1:D:434:LEU:CD2	1.96	0.79
1:C:424:LYS:HD2	1:C:425:LYS:HB2	1.64	0.79
1:B:11:TRP:N	1:B:61:ILE:HD11	1.96	0.79
1:B:98:VAL:O	1:B:105:ILE:CG1	2.29	0.79
1:C:91:TYR:CB	1:C:94:THR:HG22	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLU:HG3	1:B:67:ARG:HH12	1.45	0.79
1:B:387:LEU:HD21	1:B:434:LEU:HD21	1.65	0.79
1:B:42:ASP:HB3	1:B:43:LYS:HE3	1.64	0.79
1:B:32:THR:HG23	1:B:34:ILE:H	1.48	0.78
1:D:81:THR:HG22	1:D:278:LYS:HD3	1.66	0.78
1:C:106:ALA:CB	1:C:265:ALA:O	2.28	0.78
1:A:285:LEU:HD12	1:A:285:LEU:O	1.84	0.78
1:C:91:TYR:N	1:C:306:LYS:HE3	1.99	0.78
1:B:8:LEU:CD2	1:B:273:ASN:ND2	2.46	0.78
1:B:263:LEU:HD23	1:B:263:LEU:H	1.49	0.77
1:D:52:ALA:C	1:D:54:THR:H	1.93	0.77
1:A:32:THR:O	1:A:34:ILE:HG12	1.85	0.77
1:B:66:ASP:OD1	1:B:66:ASP:N	2.18	0.77
1:B:110:ALA:HA	1:B:303:VAL:HA	1.67	0.77
1:B:11:TRP:CH2	1:B:58:PRO:CD	2.62	0.77
1:A:60:ILE:CD1	1:A:277:ALA:HB1	2.02	0.76
1:D:133:ILE:HG13	1:D:134:PRO:HD3	1.66	0.76
1:C:89:LYS:O	1:C:306:LYS:HD2	1.86	0.76
1:B:179:ILE:HG13	1:B:334:ILE:HD12	1.67	0.75
1:B:80:ILE:HD12	1:B:107:TYR:OH	1.86	0.75
1:B:80:ILE:HD12	1:B:107:TYR:CE1	2.21	0.75
1:B:60:ILE:HG22	1:B:267:ILE:CG2	2.16	0.75
1:A:128:LYS:HE2	1:A:247:VAL:HG11	1.69	0.75
1:A:398:LEU:HD12	1:A:398:LEU:O	1.87	0.75
1:A:422:MET:O	1:A:423:LYS:HD3	1.86	0.74
1:D:433:MET:N	1:D:433:MET:HE2	2.01	0.74
1:B:11:TRP:CB	1:B:61:ILE:CD1	2.52	0.74
1:A:7:LYS:HD2	1:A:35:LYS:HE3	1.69	0.74
1:D:434:LEU:H	1:D:434:LEU:HD23	1.50	0.74
1:A:49:PRO:HA	1:A:76:LEU:HD13	1.67	0.74
1:B:48:PHE:HA	1:B:51:VAL:HG12	1.68	0.74
1:D:161:LEU:HD23	1:D:196:LEU:HD12	1.67	0.74
1:A:106:ALA:HB1	1:A:265:ALA:O	1.87	0.74
1:C:94:THR:O	1:C:108:PRO:HG3	1.87	0.74
1:B:60:ILE:HA	1:B:267:ILE:HA	1.70	0.74
1:C:65:HIS:CD2	1:C:262:VAL:HG22	2.23	0.74
1:B:22:ALA:HB2	1:B:38:VAL:HG11	1.69	0.73
1:C:385:GLU:OE2	1:C:411:ARG:NH1	2.21	0.73
1:C:47:LYS:O	1:C:51:VAL:HG22	1.88	0.73
1:B:80:ILE:O	1:B:82:PRO:HD3	1.89	0.73
1:C:406:PHE:O	1:C:414:LYS:NZ	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:TRP:CG	1:C:64:ALA:H	2.05	0.72
1:C:106:ALA:HB1	1:C:265:ALA:C	2.14	0.72
1:C:308:TYR:HA	1:C:311:GLU:CD	2.15	0.72
1:C:63:TRP:CG	1:C:64:ALA:N	2.58	0.72
1:A:11:TRP:CG	1:A:58:PRO:HG3	2.25	0.71
1:C:92:PRO:HD3	1:C:306:LYS:HZ1	1.53	0.71
1:C:143:LYS:H	1:C:143:LYS:HZ3	1.38	0.71
1:A:410:GLU:N	1:A:410:GLU:OE2	2.20	0.71
1:C:46:GLU:C	1:C:49:PRO:HD2	2.14	0.71
1:A:176:LYS:NZ	1:A:179:ILE:HG23	2.06	0.71
1:C:302:ALA:HB1	1:C:322:MET:HE2	1.71	0.71
1:C:82:PRO:HB3	1:C:107:TYR:HE1	1.55	0.71
1:C:98:VAL:HG11	1:C:106:ALA:O	1.91	0.71
1:A:285:LEU:HD12	1:A:285:LEU:C	2.16	0.71
1:A:60:ILE:HA	1:A:266:GLY:O	1.91	0.70
1:C:21:LEU:HD23	1:C:38:VAL:CG2	2.21	0.70
1:C:80:ILE:CG2	1:C:107:TYR:CZ	2.75	0.70
1:D:42:ASP:O	1:D:47:LYS:NZ	2.21	0.70
1:D:24:VAL:HG23	1:D:28:PHE:CD2	2.25	0.70
1:C:63:TRP:HD1	1:C:64:ALA:CA	2.05	0.70
1:D:29:GLU:O	1:D:33:GLY:N	2.24	0.70
1:D:41:PRO:HB2	1:D:47:LYS:HZ1	1.57	0.70
1:D:433:MET:HE3	1:D:433:MET:O	1.92	0.70
1:B:329:GLU:HG3	1:B:330:ILE:H	1.57	0.70
1:C:298:LYS:NZ	1:C:300:LEU:HA	2.07	0.70
1:B:29:GLU:OE1	1:B:35:LYS:HA	1.93	0.69
1:A:186:ASN:OD1	1:A:187:ALA:N	2.26	0.69
1:B:16:LYS:HG2	1:B:300:LEU:HD23	1.73	0.69
1:B:11:TRP:HB2	1:B:61:ILE:CG1	2.22	0.69
1:C:77:LEU:HD23	1:C:105:ILE:HD11	1.74	0.69
1:D:60:ILE:HG12	1:D:267:ILE:HG22	1.74	0.69
1:D:52:ALA:C	1:D:54:THR:N	2.49	0.69
1:D:435:LEU:O	1:D:437:THR:N	2.26	0.68
1:D:433:MET:HE2	1:D:433:MET:H	1.59	0.68
1:A:165:ASP:O	1:A:188:GLY:HA3	1.93	0.68
1:B:170:PHE:HE2	1:B:334:ILE:HG13	1.59	0.68
1:D:171:LYS:HG3	1:D:330:ILE:CG1	2.23	0.68
1:B:65:HIS:CE1	1:B:331:MET:CB	2.77	0.68
1:C:44:LEU:C	1:C:44:LEU:HD23	2.19	0.68
1:C:80:ILE:HD11	1:C:105:ILE:O	1.94	0.68
1:B:100:TYR:C	1:B:102:GLY:H	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:O	1:B:271:SER:HB3	1.93	0.68
1:D:24:VAL:CG2	1:D:28:PHE:HB3	2.19	0.67
1:D:101:ASN:O	1:D:103:LYS:HD2	1.94	0.67
1:B:335:PRO:C	1:B:337:MET:H	2.00	0.67
1:C:79:GLU:OE2	1:C:103:LYS:HD2	1.94	0.67
1:D:228:ASN:HD22	1:D:229:GLY:N	1.91	0.67
1:B:12:ILE:HG22	1:B:13:ASN:N	2.10	0.67
1:B:273:ASN:N	1:B:273:ASN:OD1	2.23	0.67
1:A:389:LYS:HB3	1:D:372:LEU:HD12	1.77	0.67
1:C:377:GLN:HG2	1:C:380:LYS:HD2	1.76	0.67
1:A:80:ILE:HB	1:A:104:LEU:HB2	1.77	0.66
1:A:82:PRO:HG2	1:A:104:LEU:HD12	1.75	0.66
1:D:44:LEU:HA	1:D:47:LYS:HE2	1.76	0.66
1:B:99:ARG:NH1	1:B:99:ARG:HA	2.10	0.66
1:B:103:LYS:HD2	1:B:103:LYS:N	2.09	0.66
1:C:71:TYR:HB3	1:C:77:LEU:HD22	1.77	0.66
1:A:278:LYS:O	1:A:282:GLU:HG3	1.96	0.66
1:C:308:TYR:HA	1:C:311:GLU:OE1	1.96	0.66
1:A:89:LYS:NZ	1:A:307:SER:H	1.94	0.65
1:D:18:TYR:HD1	1:D:19:ASN:H	1.43	0.65
1:A:106:ALA:CB	1:A:265:ALA:O	2.45	0.65
1:A:399:LYS:HA	1:A:403:LYS:CB	2.27	0.65
1:A:8:LEU:CB	1:A:36:VAL:CG1	2.63	0.65
1:A:97:ALA:HA	1:A:330:ILE:HG21	1.78	0.65
1:D:88:ASP:O	1:D:306:LYS:NZ	2.29	0.65
1:C:95:TRP:O	1:C:98:VAL:N	2.30	0.65
1:D:119:ASN:HD21	1:D:122:LEU:HD23	1.61	0.65
1:D:336:GLN:C	1:D:338:SER:H	2.05	0.65
1:A:45:GLU:OE2	1:A:45:GLU:N	2.29	0.65
1:D:16:LYS:NZ	1:D:63:TRP:HZ3	1.94	0.65
1:B:111:VAL:HG11	1:B:322:MET:SD	2.37	0.65
1:B:59:ASP:O	1:B:268:ASN:N	2.20	0.64
1:A:5:GLU:HB2	1:A:273:ASN:CG	2.23	0.64
1:B:89:LYS:O	1:B:305:LEU:HD23	1.97	0.64
1:B:154:GLU:HG3	1:B:156:TYR:H	1.63	0.64
1:D:271:SER:OG	1:D:272:PRO:HD2	1.96	0.64
1:B:26:LYS:NZ	1:B:30:LYS:HD3	2.12	0.64
1:C:80:ILE:CG2	1:C:107:TYR:OH	2.45	0.64
1:D:376:GLU:OE2	1:D:377:GLN:NE2	2.30	0.64
1:A:29:GLU:HG2	1:A:29:GLU:O	1.96	0.64
1:A:395:VAL:HG13	1:A:396:LEU:HG	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLY:HA3	1:C:294:VAL:HA	1.78	0.64
1:D:81:THR:HG22	1:D:278:LYS:CD	2.28	0.64
1:D:165:ASP:OD1	1:D:254:GLN:NE2	2.30	0.64
1:D:273:ASN:HB3	1:D:276:LEU:HD23	1.79	0.64
1:B:60:ILE:CG2	1:B:267:ILE:HG23	2.23	0.64
1:C:78:ALA:HB2	1:C:269:ALA:HA	1.80	0.64
1:C:141:LYS:HD2	1:C:141:LYS:O	1.97	0.64
1:B:17:GLY:HA3	1:B:297:ASP:HB3	1.79	0.64
1:C:13:ASN:HD21	1:C:63:TRP:HZ3	1.45	0.64
1:C:295:ASN:OD1	1:C:300:LEU:N	2.28	0.63
1:D:302:ALA:HB1	1:D:322:MET:HE2	1.78	0.63
1:D:434:LEU:C	1:D:436:GLN:H	2.05	0.63
1:C:10:ILE:HG12	1:C:60:ILE:HB	1.79	0.63
1:D:409:ALA:O	1:D:414:LYS:NZ	2.32	0.63
1:C:63:TRP:CD1	1:C:64:ALA:CA	2.81	0.63
1:C:305:LEU:HD23	1:C:308:TYR:H	1.64	0.63
1:B:367:THR:HA	1:B:370:VAL:HG12	1.81	0.63
1:D:19:ASN:HA	1:D:22:ALA:HB3	1.81	0.63
1:B:433:MET:HA	1:B:436:GLN:OE1	1.99	0.63
1:A:257:LYS:NZ	1:A:329:GLU:OE2	2.32	0.62
1:C:123:LEU:HD22	1:C:124:PRO:HD2	1.81	0.62
1:D:435:LEU:C	1:D:437:THR:H	2.05	0.62
1:A:201:LYS:NZ	1:A:352:ALA:O	2.20	0.62
1:C:91:TYR:CG	1:C:306:LYS:HE2	2.32	0.62
1:B:13:ASN:HD21	1:B:15:ASP:CG	2.07	0.62
1:C:311:GLU:OE2	1:C:311:GLU:N	2.19	0.62
1:D:72:ALA:HB3	1:D:100:TYR:HE2	1.65	0.62
1:A:277:ALA:O	1:A:280:PHE:N	2.33	0.61
1:B:11:TRP:C	1:B:61:ILE:HD11	2.25	0.61
1:B:168:TYR:OH	1:B:171:LYS:NZ	2.26	0.61
1:C:245:VAL:HB	1:C:317:ARG:HA	1.82	0.61
1:D:400:GLU:O	1:D:403:LYS:N	2.26	0.61
1:A:77:LEU:O	1:A:269:ALA:HB2	2.00	0.61
1:B:64:ALA:O	1:B:68:PHE:CD1	2.54	0.61
1:D:52:ALA:O	1:D:55:GLY:N	2.31	0.61
1:A:176:LYS:HZ3	1:A:179:ILE:HG23	1.66	0.61
1:A:389:LYS:NZ	1:A:392:GLN:OE1	2.29	0.61
1:C:91:TYR:HA	1:C:306:LYS:NZ	2.14	0.61
1:B:100:TYR:O	1:B:102:GLY:N	2.34	0.61
1:C:90:LEU:HD22	1:C:304:ALA:C	2.26	0.61
1:A:284:TYR:C	1:A:287:THR:HG23	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLU:OE1	1:B:103:LYS:CG	2.45	0.61
1:C:98:VAL:O	1:C:105:ILE:HG22	2.01	0.61
1:C:298:LYS:HD2	1:C:299:PRO:HD2	1.81	0.61
1:B:80:ILE:O	1:B:82:PRO:CD	2.49	0.60
1:D:160:PRO:HG3	1:D:258:PRO:HA	1.83	0.60
1:B:131:GLU:OE2	1:B:131:GLU:N	2.34	0.60
1:C:25:GLY:O	1:C:28:PHE:HB3	1.99	0.60
1:D:273:ASN:HB3	1:D:276:LEU:HB2	1.82	0.60
1:B:90:LEU:C	1:B:306:LYS:HE3	2.27	0.60
1:B:368:ASN:HD21	1:D:367:THR:HG21	1.65	0.60
1:C:186:ASN:OD1	1:C:189:ALA:N	2.33	0.60
1:C:296:LYS:HE3	1:C:297:ASP:HB2	1.83	0.60
1:C:65:HIS:CE1	1:C:97:ALA:HB1	2.36	0.60
1:D:219:ASN:HD21	1:D:235:ASN:HB3	1.66	0.60
1:B:87:GLN:O	1:B:87:GLN:HG2	2.01	0.60
1:A:77:LEU:HD12	1:A:105:ILE:HG23	1.83	0.60
1:D:411:ARG:HA	1:D:414:LYS:HE2	1.83	0.60
1:A:411:ARG:HA	1:A:414:LYS:HG3	1.84	0.59
1:C:65:HIS:CD2	1:C:262:VAL:H	2.20	0.59
1:A:11:TRP:HB2	1:A:61:ILE:HG22	1.84	0.59
1:D:285:LEU:O	1:D:291:LEU:HG	2.02	0.59
1:C:305:LEU:CD2	1:C:307:SER:OG	2.37	0.59
1:B:303:VAL:O	1:B:309:GLU:HB2	2.01	0.59
1:C:40:HIS:O	1:C:40:HIS:ND1	2.35	0.59
1:D:111:VAL:HG12	1:D:262:VAL:HG13	1.83	0.59
1:C:80:ILE:HG21	1:C:107:TYR:CZ	2.38	0.59
1:A:107:TYR:HE2	1:A:282:GLU:OE2	1.86	0.59
1:B:263:LEU:HD23	1:B:263:LEU:N	2.18	0.59
1:C:119:ASN:HA	1:C:243:TYR:HA	1.84	0.59
1:B:335:PRO:C	1:B:337:MET:N	2.56	0.58
1:D:15:ASP:OD1	1:D:15:ASP:N	2.31	0.58
1:A:6:GLY:H	1:A:273:ASN:HD21	1.49	0.58
1:A:11:TRP:CD2	1:A:58:PRO:HG3	2.38	0.58
1:A:273:ASN:HB3	1:A:276:LEU:HB2	1.85	0.58
1:A:423:LYS:NZ	1:A:433:MET:SD	2.76	0.58
1:A:440:SER:O	1:D:380:LYS:NZ	2.35	0.58
1:B:98:VAL:HG12	1:B:98:VAL:O	2.03	0.58
1:A:10:ILE:HG21	1:A:21:LEU:HD23	1.84	0.58
1:D:336:GLN:C	1:D:338:SER:N	2.61	0.58
1:D:16:LYS:NZ	1:D:63:TRP:CZ3	2.71	0.58
1:C:110:ALA:HA	1:C:303:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ASN:HA	1:C:414:LYS:NZ	2.19	0.58
1:A:89:LYS:HZ3	1:A:307:SER:H	1.52	0.57
1:B:90:LEU:HG	1:B:305:LEU:HA	1.86	0.57
1:C:60:ILE:HG12	1:C:267:ILE:HG22	1.86	0.57
1:A:190:LYS:O	1:A:194:THR:HG23	2.05	0.57
1:A:194:THR:HG22	1:A:358:VAL:HG21	1.86	0.57
1:C:305:LEU:CD2	1:C:308:TYR:H	2.17	0.57
1:D:309:GLU:HA	1:D:312:LEU:CD1	2.33	0.57
1:A:117:ILE:HG23	1:A:245:VAL:HG12	1.86	0.57
1:C:86:PHE:CE2	1:C:282:GLU:HG2	2.39	0.57
1:D:117:ILE:HG12	1:D:245:VAL:HG12	1.87	0.57
1:A:28:PHE:CD2	1:A:32:THR:HG21	2.39	0.57
1:B:12:ILE:CG2	1:B:13:ASN:N	2.68	0.57
1:B:257:LYS:HB3	1:B:328:GLY:HA2	1.85	0.57
1:D:66:ASP:O	1:D:67:ARG:HG3	2.04	0.57
1:D:96:ASP:HA	1:D:99:ARG:HB3	1.86	0.57
1:A:65:HIS:HE1	1:A:261:GLY:HA2	1.70	0.57
1:A:176:LYS:HZ1	1:A:179:ILE:H	1.52	0.57
1:C:108:PRO:HA	1:C:264:SER:HA	1.87	0.57
1:C:109:ILE:O	1:C:304:ALA:N	2.34	0.57
1:A:32:THR:O	1:A:34:ILE:N	2.37	0.57
1:B:65:HIS:HE1	1:B:331:MET:CB	2.17	0.57
1:B:275:GLU:O	1:B:278:LYS:N	2.37	0.57
1:B:330:ILE:H	1:B:330:ILE:HD12	1.70	0.56
1:C:34:ILE:HG13	1:C:276:LEU:HD13	1.86	0.56
1:A:8:LEU:O	1:A:36:VAL:HA	2.04	0.56
1:A:81:THR:OG1	1:A:278:LYS:NZ	2.25	0.56
1:B:45:GLU:CG	1:B:67:ARG:HH12	2.16	0.56
1:B:329:GLU:HG3	1:B:330:ILE:N	2.20	0.56
1:B:383:LEU:HD21	1:B:434:LEU:HD22	1.85	0.56
1:D:17:GLY:HA2	1:D:298:LYS:HE3	1.86	0.56
1:A:398:LEU:HD12	1:A:398:LEU:C	2.30	0.56
1:B:76:LEU:O	1:B:269:ALA:HB2	2.06	0.56
1:A:6:GLY:O	1:A:34:ILE:HD12	2.05	0.56
1:A:118:TYR:CE1	1:A:126:PRO:HG3	2.41	0.56
1:C:141:LYS:O	1:C:144:GLY:N	2.39	0.56
1:D:172:TYR:CD1	1:D:172:TYR:N	2.73	0.56
1:B:9:VAL:O	1:B:60:ILE:HG12	2.06	0.56
1:B:12:ILE:CD1	1:B:62:PHE:CB	2.83	0.56
1:C:92:PRO:HD3	1:C:306:LYS:HZ3	1.68	0.56
1:D:308:TYR:CD2	1:D:312:LEU:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:HB3	1:B:262:VAL:O	2.06	0.56
1:B:390:LEU:H	1:B:390:LEU:HD23	1.70	0.56
1:C:119:ASN:HD21	1:C:122:LEU:HG	1.70	0.56
1:A:82:PRO:HG2	1:A:104:LEU:CD1	2.34	0.56
1:B:89:LYS:O	1:B:306:LYS:HG3	2.06	0.56
1:B:439:PHE:CE2	1:C:383:LEU:HD21	2.40	0.56
1:C:95:TRP:O	1:C:99:ARG:N	2.33	0.56
1:D:22:ALA:HB2	1:D:38:VAL:HG22	1.88	0.56
1:A:22:ALA:O	1:A:26:LYS:N	2.31	0.56
1:B:42:ASP:HB3	1:B:43:LYS:CE	2.36	0.56
1:B:13:ASN:CG	1:B:15:ASP:H	2.14	0.55
1:B:186:ASN:OD1	1:B:188:GLY:N	2.28	0.55
1:D:52:ALA:CB	1:D:268:ASN:ND2	2.57	0.55
1:D:434:LEU:O	1:D:436:GLN:N	2.39	0.55
1:A:277:ALA:O	1:A:279:GLU:N	2.39	0.55
1:C:130:TRP:CD1	1:C:249:PRO:HB2	2.41	0.55
1:D:163:ALA:O	1:D:257:LYS:NZ	2.31	0.55
1:D:308:TYR:C	1:D:312:LEU:CD1	2.78	0.55
1:A:176:LYS:HZ1	1:A:179:ILE:N	2.04	0.55
1:D:48:PHE:CD1	1:D:48:PHE:C	2.85	0.55
1:B:8:LEU:HD21	1:B:273:ASN:ND2	2.21	0.55
1:C:311:GLU:CD	1:C:311:GLU:H	2.09	0.55
1:C:378:LEU:HD21	1:D:382:VAL:HG12	1.87	0.55
1:D:433:MET:O	1:D:433:MET:HG2	2.04	0.55
1:B:8:LEU:CD2	1:B:273:ASN:CB	2.78	0.55
1:B:100:TYR:C	1:B:102:GLY:N	2.65	0.55
1:B:179:ILE:CG1	1:B:334:ILE:HD12	2.33	0.55
1:D:435:LEU:C	1:D:437:THR:N	2.64	0.55
1:B:90:LEU:HD23	1:B:304:ALA:HB3	1.88	0.54
1:C:90:LEU:HD22	1:C:304:ALA:O	2.07	0.54
1:C:143:LYS:H	1:C:143:LYS:NZ	2.05	0.54
1:B:434:LEU:HA	1:B:437:THR:HG22	1.89	0.54
1:C:50:GLN:HG3	1:C:423:LYS:CE	2.37	0.54
1:D:271:SER:OG	1:D:272:PRO:CD	2.55	0.54
1:D:312:LEU:HD12	1:D:312:LEU:H	1.72	0.54
1:B:80:ILE:C	1:B:82:PRO:HD3	2.31	0.54
1:B:292:GLU:OE2	1:B:296:LYS:HG3	2.08	0.54
1:C:21:LEU:HA	1:C:24:VAL:HG12	1.89	0.54
1:C:91:TYR:CZ	1:C:306:LYS:HG2	2.42	0.54
1:C:109:ILE:HD12	1:C:109:ILE:N	2.22	0.54
1:D:138:LYS:O	1:D:139:GLU:C	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:HD12	1:D:389:LYS:HG2	1.90	0.54
1:B:110:ALA:CB	1:B:263:LEU:HD21	2.34	0.54
1:B:78:ALA:HB2	1:B:269:ALA:HA	1.88	0.54
1:B:160:PRO:HG3	1:B:258:PRO:HA	1.89	0.54
1:C:308:TYR:HA	1:C:311:GLU:OE2	2.08	0.54
1:C:298:LYS:NZ	1:C:300:LEU:HD23	2.23	0.54
1:A:65:HIS:CE1	1:A:261:GLY:HA2	2.42	0.54
1:D:65:HIS:N	1:D:262:VAL:O	2.35	0.54
1:A:12:ILE:HG13	1:A:62:PHE:HB2	1.90	0.54
1:A:268:ASN:OD1	1:A:269:ALA:N	2.41	0.54
1:B:43:LYS:HE2	1:B:43:LYS:N	2.23	0.54
1:C:42:ASP:OD1	1:C:42:ASP:N	2.37	0.54
1:A:49:PRO:HA	1:A:76:LEU:CD1	2.36	0.53
1:B:31:ASP:OD1	1:B:284:TYR:OH	2.26	0.53
1:B:184:VAL:HG12	1:B:362:LEU:HD12	1.90	0.53
1:A:302:ALA:HB1	1:A:322:MET:HE2	1.90	0.53
1:B:206:ASN:OD1	1:B:208:ASP:N	2.22	0.53
1:C:399:LYS:HZ2	1:C:401:GLU:HB2	1.73	0.53
1:D:51:VAL:O	1:D:56:ASP:C	2.51	0.53
1:A:394:ASN:OD1	1:A:403:LYS:NZ	2.42	0.53
1:B:71:TYR:N	1:B:71:TYR:CD1	2.75	0.53
1:C:232:ALA:O	1:C:236:ILE:HG13	2.09	0.53
1:B:65:HIS:HE1	1:B:260:VAL:O	1.87	0.53
1:B:79:GLU:OE1	1:B:103:LYS:CB	2.56	0.53
1:D:133:ILE:HA	1:D:136:LEU:HG	1.91	0.53
1:D:388:GLU:O	1:D:392:GLN:HG2	2.09	0.53
1:B:3:ILE:N	1:B:56:ASP:OD1	2.42	0.53
1:C:160:PRO:HG3	1:C:258:PRO:HA	1.91	0.53
1:D:48:PHE:C	1:D:50:GLN:H	2.16	0.53
1:A:77:LEU:C	1:A:269:ALA:HB2	2.34	0.52
1:B:20:GLY:O	1:B:24:VAL:HG12	2.09	0.52
1:C:23:GLU:O	1:C:27:LYS:HG3	2.09	0.52
1:C:64:ALA:HA	1:C:263:LEU:HA	1.91	0.52
1:C:308:TYR:O	1:C:308:TYR:CG	2.62	0.52
1:D:268:ASN:OD1	1:D:269:ALA:N	2.42	0.52
1:A:60:ILE:HD13	1:A:281:LEU:HD11	1.90	0.52
1:B:99:ARG:NH1	1:B:99:ARG:CA	2.73	0.52
1:D:284:TYR:O	1:D:290:GLY:HA3	2.10	0.52
1:B:9:VAL:HG22	1:B:10:ILE:N	2.23	0.52
1:B:99:ARG:HB2	1:B:99:ARG:NH1	2.24	0.52
1:B:345:ARG:HH22	1:C:429:LYS:CD	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LYS:O	1:C:306:LYS:CD	2.56	0.52
1:C:89:LYS:NZ	1:C:305:LEU:HD11	2.24	0.52
1:D:140:LEU:HD23	1:D:224:ALA:HB2	1.91	0.52
1:D:340:PHE:O	1:D:344:VAL:HG22	2.10	0.52
1:B:48:PHE:HB3	1:B:49:PRO:HD3	1.91	0.52
1:C:80:ILE:HG22	1:C:82:PRO:HD3	1.91	0.52
1:C:430:VAL:HG22	1:C:432:GLU:H	1.74	0.52
1:B:79:GLU:HG2	1:B:80:ILE:H	1.75	0.52
1:D:25:GLY:O	1:D:30:LYS:HE3	2.09	0.52
1:D:245:VAL:HG23	1:D:320:ALA:HB3	1.91	0.52
1:B:45:GLU:CG	1:B:67:ARG:NH1	2.58	0.52
1:C:11:TRP:CE3	1:C:58:PRO:HD3	2.44	0.52
1:B:76:LEU:O	1:B:269:ALA:CB	2.58	0.52
1:B:286:LEU:O	1:B:305:LEU:CD1	2.55	0.52
1:C:419:VAL:HG23	1:C:422:MET:SD	2.50	0.52
1:D:24:VAL:HG23	1:D:28:PHE:CG	2.44	0.52
1:A:383:LEU:O	1:A:387:LEU:HD12	2.11	0.51
1:B:11:TRP:CA	1:B:61:ILE:CD1	2.66	0.51
1:D:81:THR:HG23	1:D:81:THR:O	2.10	0.51
1:D:119:ASN:ND2	1:D:122:LEU:HD23	2.26	0.51
1:A:81:THR:CB	1:A:278:LYS:HZ3	2.19	0.51
1:A:87:GLN:HG2	1:A:95:TRP:CE2	2.45	0.51
1:D:261:GLY:HA2	1:D:331:MET:HE3	1.93	0.51
1:A:288:ASP:OD1	1:A:307:SER:OG	2.27	0.51
1:C:184:VAL:HG21	1:C:344:VAL:HG22	1.91	0.51
1:D:41:PRO:HB2	1:D:47:LYS:NZ	2.26	0.51
1:D:433:MET:H	1:D:433:MET:CE	2.22	0.51
1:A:278:LYS:O	1:A:282:GLU:CG	2.58	0.51
1:B:45:GLU:HB3	1:B:63:TRP:HE1	1.75	0.51
1:C:90:LEU:HD23	1:C:305:LEU:HA	1.92	0.51
1:C:159:TRP:HZ3	1:C:184:VAL:HG23	1.75	0.51
1:A:155:PRO:HD3	1:A:345:ARG:HB2	1.92	0.51
1:B:48:PHE:HA	1:B:51:VAL:CG1	2.39	0.51
1:B:263:LEU:H	1:B:263:LEU:CD2	2.21	0.51
1:B:322:MET:HG3	1:B:326:GLN:HE21	1.75	0.51
1:D:406:PHE:CE2	1:D:418:PHE:HB2	2.46	0.51
1:C:129:THR:HA	1:C:250:THR:H	1.76	0.51
1:B:8:LEU:HD21	1:B:273:ASN:CG	2.34	0.51
1:B:103:LYS:N	1:B:103:LYS:CD	2.73	0.51
1:B:370:VAL:O	1:B:374:VAL:HG13	2.11	0.51
1:A:389:LYS:CB	1:D:372:LEU:HD12	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:HA	1:B:32:THR:HG22	1.92	0.51
1:C:301:GLY:O	1:C:318:ILE:HD11	2.11	0.51
1:C:44:LEU:HG	1:C:44:LEU:O	2.10	0.50
1:B:434:LEU:HA	1:B:437:THR:CG2	2.42	0.50
1:C:87:GLN:O	1:C:88:ASP:CB	2.43	0.50
1:A:118:TYR:CE2	1:A:120:LYS:HG2	2.46	0.50
1:D:405:LYS:NZ	1:D:420:ASP:OD2	2.43	0.50
1:A:68:PHE:HB3	1:A:105:ILE:HG21	1.93	0.50
1:B:331:MET:HG3	1:B:332:PRO:HD2	1.93	0.50
1:C:383:LEU:O	1:C:387:LEU:HD12	2.11	0.50
1:A:24:VAL:HG13	1:A:293:ALA:HB3	1.93	0.50
1:C:140:LEU:HA	1:C:143:LYS:CE	2.42	0.50
1:D:226:THR:HG22	1:D:227:ILE:H	1.76	0.50
1:D:419:VAL:HG12	1:D:419:VAL:O	2.12	0.50
1:A:170:PHE:HB3	1:A:177:TYR:HB3	1.92	0.50
1:C:305:LEU:HD23	1:C:307:SER:N	2.27	0.50
1:C:343:ALA:HB2	1:C:369:ALA:HB2	1.93	0.50
1:B:9:VAL:HG23	1:B:37:THR:OG1	2.11	0.50
1:B:98:VAL:CG1	1:B:105:ILE:CG1	2.66	0.49
1:C:312:LEU:O	1:C:315:ASP:N	2.45	0.49
1:C:50:GLN:HG3	1:C:423:LYS:NZ	2.27	0.49
1:D:434:LEU:C	1:D:436:GLN:N	2.65	0.49
1:B:11:TRP:O	1:B:61:ILE:HD11	2.12	0.49
1:C:48:PHE:HD2	1:C:71:TYR:CZ	2.30	0.49
1:C:106:ALA:CB	1:C:266:GLY:HA2	2.36	0.49
1:D:52:ALA:HB1	1:D:268:ASN:HD21	1.72	0.49
1:B:59:ASP:HA	1:B:271:SER:HB2	1.95	0.49
1:A:28:PHE:CE1	1:A:280:PHE:HD1	2.30	0.49
1:A:232:ALA:O	1:A:236:ILE:HG13	2.12	0.49
1:C:296:LYS:HD2	1:C:296:LYS:C	2.37	0.49
1:B:387:LEU:HA	1:B:390:LEU:HD21	1.93	0.49
1:C:91:TYR:CA	1:C:306:LYS:CE	2.69	0.49
1:D:137:ASP:O	1:D:141:LYS:N	2.45	0.49
1:D:312:LEU:HD12	1:D:312:LEU:N	2.27	0.49
1:C:80:ILE:HG22	1:C:107:TYR:OH	2.12	0.49
1:D:52:ALA:C	1:D:55:GLY:H	2.21	0.49
1:A:305:LEU:HD21	1:A:307:SER:OG	2.12	0.49
1:C:98:VAL:HG13	1:C:105:ILE:CG2	2.36	0.49
1:D:47:LYS:N	1:D:49:PRO:HD3	2.28	0.49
1:D:52:ALA:O	1:D:54:THR:N	2.45	0.49
1:B:11:TRP:O	1:B:61:ILE:CD1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:CZ	1:B:99:ARG:CB	2.85	0.49
1:D:418:PHE:CD1	1:D:418:PHE:C	2.91	0.49
1:A:398:LEU:C	1:A:398:LEU:CD1	2.85	0.48
1:B:45:GLU:HB3	1:B:63:TRP:NE1	2.27	0.48
1:C:129:THR:HA	1:C:250:THR:N	2.28	0.48
1:C:333:ASN:OD1	1:C:333:ASN:O	2.31	0.48
1:B:345:ARG:NH2	1:C:395:VAL:O	2.46	0.48
1:C:65:HIS:HD2	1:C:262:VAL:H	1.59	0.48
1:C:95:TRP:O	1:C:96:ASP:C	2.56	0.48
1:C:108:PRO:C	1:C:109:ILE:HD12	2.38	0.48
1:C:158:THR:O	1:C:162:ILE:HG12	2.12	0.48
1:D:139:GLU:N	1:D:139:GLU:CD	2.71	0.48
1:C:11:TRP:HA	1:C:39:GLU:O	2.13	0.48
1:A:171:LYS:O	1:A:178:ASP:N	2.37	0.48
1:B:8:LEU:O	1:B:36:VAL:HA	2.14	0.48
1:B:150:PHE:CE1	1:B:205:MET:HE1	2.48	0.48
1:C:298:LYS:NZ	1:C:299:PRO:O	2.43	0.48
1:C:378:LEU:CD2	1:D:382:VAL:HG12	2.43	0.48
1:A:60:ILE:HG12	1:A:267:ILE:HG13	1.95	0.48
1:A:82:PRO:CG	1:A:104:LEU:HD12	2.43	0.48
1:B:11:TRP:CZ2	1:B:58:PRO:HD3	2.39	0.48
1:C:141:LYS:HD2	1:C:144:GLY:HA2	1.96	0.48
1:A:28:PHE:CZ	1:A:280:PHE:CD1	3.02	0.48
1:B:21:LEU:O	1:B:25:GLY:N	2.47	0.48
1:D:401:GLU:HA	1:D:404:GLN:CD	2.36	0.48
1:C:314:LYS:O	1:C:314:LYS:HD3	2.14	0.48
1:C:331:MET:SD	1:C:332:PRO:HD2	2.54	0.48
1:C:407:ASN:HA	1:C:414:LYS:HZ2	1.77	0.48
1:D:94:THR:HG22	1:D:111:VAL:HG11	1.96	0.48
1:D:219:ASN:ND2	1:D:235:ASN:HB3	2.27	0.48
1:B:99:ARG:NH1	1:B:99:ARG:CB	2.77	0.47
1:A:170:PHE:CB	1:A:177:TYR:HB3	2.43	0.47
1:B:79:GLU:CD	1:B:103:LYS:CG	2.86	0.47
1:C:141:LYS:C	1:C:144:GLY:H	2.21	0.47
1:D:152:LEU:HD11	1:D:205:MET:SD	2.54	0.47
1:A:28:PHE:CE1	1:A:280:PHE:CD1	3.03	0.47
1:C:295:ASN:HA	1:C:298:LYS:O	2.14	0.47
1:A:63:TRP:HA	1:A:63:TRP:CE3	2.50	0.47
1:C:53:ALA:HA	1:C:76:LEU:HD22	1.96	0.47
1:A:154:GLU:HG3	1:A:156:TYR:H	1.80	0.47
1:B:11:TRP:N	1:B:61:ILE:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:HG11	1:B:106:ALA:HB3	1.96	0.47
1:C:46:GLU:O	1:C:49:PRO:CG	2.61	0.47
1:C:65:HIS:CE1	1:C:330:ILE:HG23	2.31	0.47
1:C:86:PHE:CD2	1:C:282:GLU:HG2	2.50	0.47
1:C:245:VAL:HG12	1:C:320:ALA:HB3	1.96	0.47
1:D:142:ALA:C	1:D:144:GLY:H	2.22	0.47
1:D:274:LYS:O	1:D:278:LYS:HE2	2.14	0.47
1:D:331:MET:HE2	1:D:331:MET:HB2	1.72	0.47
1:A:90:LEU:HD13	1:A:108:PRO:HG2	1.97	0.47
1:B:59:ASP:O	1:B:267:ILE:HG22	2.15	0.47
1:A:32:THR:C	1:A:34:ILE:H	2.22	0.47
1:A:80:ILE:HG22	1:A:82:PRO:HD3	1.97	0.47
1:B:178:ASP:N	1:B:334:ILE:HD11	2.30	0.47
1:C:3:ILE:HG23	1:C:56:ASP:HA	1.97	0.47
1:C:193:LEU:HG	1:C:358:VAL:HG13	1.97	0.47
1:A:440:SER:H	1:D:415:ARG:HH21	1.63	0.47
1:B:9:VAL:O	1:B:10:ILE:HG13	2.13	0.47
1:A:41:PRO:O	1:A:44:LEU:HB3	2.15	0.46
1:C:308:TYR:C	1:C:311:GLU:OE2	2.58	0.46
1:D:62:PHE:HB3	1:D:263:LEU:HD11	1.96	0.46
1:A:90:LEU:HD13	1:A:108:PRO:CG	2.46	0.46
1:C:21:LEU:N	1:C:294:VAL:HG12	2.31	0.46
1:C:91:TYR:CG	1:C:306:LYS:CE	2.97	0.46
1:C:153:GLN:O	1:C:345:ARG:NH1	2.48	0.46
1:D:62:PHE:CE2	1:D:265:ALA:HB2	2.51	0.46
1:D:131:GLU:O	1:D:134:PRO:HD2	2.15	0.46
1:C:281:LEU:HA	1:C:285:LEU:HB3	1.97	0.46
1:D:65:HIS:O	1:D:65:HIS:CG	2.69	0.46
1:A:10:ILE:HD11	1:A:280:PHE:CE2	2.50	0.46
1:A:176:LYS:NZ	1:A:177:TYR:O	2.33	0.46
1:C:12:ILE:O	1:C:40:HIS:CB	2.64	0.46
1:A:10:ILE:HD11	1:A:280:PHE:HE2	1.80	0.46
1:D:153:GLN:NE2	1:D:208:ASP:HA	2.31	0.46
1:D:411:ARG:HA	1:D:414:LYS:CE	2.46	0.46
1:B:98:VAL:HA	1:B:105:ILE:HD11	1.97	0.46
1:B:99:ARG:CA	1:B:99:ARG:HH11	2.29	0.46
1:B:99:ARG:O	1:B:99:ARG:HG3	2.08	0.46
1:B:275:GLU:O	1:B:276:LEU:C	2.58	0.46
1:C:16:LYS:HE2	1:C:263:LEU:HD13	1.98	0.46
1:C:90:LEU:HB2	1:C:95:TRP:HZ2	1.74	0.46
1:D:303:VAL:HG23	1:D:309:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:LEU:HD23	1:D:434:LEU:N	2.26	0.46
1:A:11:TRP:CD1	1:A:39:GLU:HB2	2.51	0.46
1:A:48:PHE:CE2	1:A:61:ILE:HD13	2.51	0.46
1:A:413:ASP:O	1:A:417:VAL:HG12	2.16	0.46
1:A:435:LEU:O	1:A:437:THR:N	2.49	0.46
1:B:150:PHE:CD1	1:B:227:ILE:HG13	2.51	0.46
1:C:208:ASP:OD1	1:C:208:ASP:N	2.39	0.46
1:D:72:ALA:HB3	1:D:100:TYR:CE2	2.46	0.46
1:B:335:PRO:O	1:B:337:MET:N	2.49	0.46
1:B:434:LEU:HD12	1:B:434:LEU:H	1.80	0.46
1:B:442:ASP:OD2	1:C:336:GLN:HG3	2.16	0.46
1:C:312:LEU:HB3	1:C:318:ILE:HD13	1.96	0.46
1:C:10:ILE:HG21	1:C:21:LEU:HD21	1.98	0.45
1:B:65:HIS:HD1	1:B:261:GLY:HA2	1.81	0.45
1:B:344:VAL:O	1:B:348:VAL:HG23	2.16	0.45
1:B:437:THR:HG23	1:B:438:PHE:CD2	2.51	0.45
1:B:11:TRP:CH2	1:B:51:VAL:HG21	2.50	0.45
1:D:71:TYR:O	1:D:76:LEU:HB2	2.16	0.45
1:A:32:THR:C	1:A:34:ILE:N	2.73	0.45
1:A:129:THR:HG23	1:A:132:GLU:H	1.81	0.45
1:B:86:PHE:HA	1:B:89:LYS:HZ2	1.81	0.45
1:B:89:LYS:O	1:B:305:LEU:CD2	2.63	0.45
1:B:236:ILE:HD13	1:B:236:ILE:HG21	1.76	0.45
1:D:141:LYS:HA	1:D:141:LYS:HD3	1.72	0.45
1:C:116:LEU:HD22	1:C:249:PRO:HG3	1.98	0.45
1:D:48:PHE:C	1:D:50:GLN:N	2.71	0.45
1:D:65:HIS:NE2	1:D:97:ALA:O	2.47	0.45
1:D:404:GLN:CD	1:D:404:GLN:H	2.16	0.45
1:B:84:ALA:O	1:B:88:ASP:OD1	2.35	0.45
1:C:63:TRP:HD1	1:C:64:ALA:C	2.25	0.45
1:D:63:TRP:CE3	1:D:63:TRP:HA	2.51	0.45
1:A:106:ALA:HA	1:A:265:ALA:O	2.17	0.45
1:B:44:LEU:HA	1:B:44:LEU:HD12	1.49	0.45
1:C:26:LYS:O	1:C:29:GLU:HG2	2.17	0.45
1:C:144:GLY:C	1:C:145:LYS:HE2	2.42	0.45
1:C:363:ALA:O	1:C:367:THR:HG23	2.17	0.45
1:A:218:PHE:HE2	1:A:236:ILE:HD13	1.82	0.45
1:B:275:GLU:HA	1:B:278:LYS:HD3	1.99	0.45
1:D:97:ALA:HA	1:D:330:ILE:CG2	2.47	0.45
1:A:435:LEU:HB3	1:A:436:GLN:H	1.66	0.45
1:A:436:GLN:HB3	1:A:439:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LEU:O	1:C:25:GLY:N	2.49	0.45
1:D:25:GLY:HA2	1:D:29:GLU:OE1	2.16	0.45
1:D:406:PHE:CZ	1:D:414:LYS:HG2	2.52	0.45
1:D:245:VAL:HG22	1:D:317:ARG:HB3	1.99	0.44
1:D:341:TRP:O	1:D:345:ARG:HB2	2.16	0.44
1:A:28:PHE:CZ	1:A:280:PHE:HD1	2.34	0.44
1:A:422:MET:C	1:A:423:LYS:HD3	2.41	0.44
1:B:61:ILE:HD12	1:B:62:PHE:H	1.82	0.44
1:C:28:PHE:CE2	1:C:34:ILE:HB	2.53	0.44
1:C:288:ASP:CG	1:C:308:TYR:HB2	2.42	0.44
1:C:320:ALA:O	1:C:324:ASN:ND2	2.50	0.44
1:A:77:LEU:O	1:A:269:ALA:CB	2.63	0.44
1:A:158:THR:O	1:A:162:ILE:HG13	2.16	0.44
1:A:160:PRO:HG3	1:A:258:PRO:HA	1.98	0.44
1:B:309:GLU:O	1:B:313:ALA:N	2.50	0.44
1:C:92:PRO:CD	1:C:306:LYS:NZ	2.75	0.44
1:A:10:ILE:HG21	1:A:21:LEU:CD2	2.46	0.44
1:D:118:TYR:O	1:D:243:TYR:HB2	2.18	0.44
1:D:178:ASP:C	1:D:179:ILE:HG12	2.42	0.44
1:A:236:ILE:O	1:A:239:SER:OG	2.28	0.44
1:B:97:ALA:HA	1:B:330:ILE:HG21	2.00	0.44
1:C:399:LYS:NZ	1:C:401:GLU:HB2	2.33	0.44
1:D:16:LYS:N	1:D:16:LYS:HD2	2.33	0.44
1:A:7:LYS:CD	1:A:35:LYS:HE3	2.44	0.44
1:B:3:ILE:HG13	1:B:4:GLU:N	2.33	0.44
1:B:107:TYR:HB3	1:B:286:LEU:HD11	1.99	0.44
1:D:377:GLN:HA	1:D:380:LYS:HB2	1.98	0.44
1:A:184:VAL:HG11	1:A:344:VAL:HG22	2.00	0.44
1:A:60:ILE:CG2	1:A:265:ALA:HB1	2.48	0.44
1:B:182:VAL:HG13	1:B:340:PHE:HA	2.00	0.44
1:C:389:LYS:NZ	1:D:371:ASP:OD2	2.44	0.44
1:D:433:MET:N	1:D:433:MET:CE	2.77	0.44
1:A:109:ILE:HG12	1:A:264:SER:HA	2.00	0.43
1:B:123:LEU:HD21	1:B:136:LEU:HD21	2.00	0.43
1:D:402:ASP:OD2	1:D:421:ALA:HB2	2.18	0.43
1:A:90:LEU:HD12	1:A:95:TRP:CZ2	2.53	0.43
1:A:176:LYS:HD2	1:A:177:TYR:N	2.32	0.43
1:B:79:GLU:HG2	1:B:80:ILE:N	2.33	0.43
1:C:139:GLU:O	1:C:143:LYS:NZ	2.35	0.43
1:B:99:ARG:NH1	1:B:103:LYS:O	2.52	0.43
1:B:383:LEU:HD21	1:B:434:LEU:CD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LYS:HE2	1:C:43:LYS:H	1.83	0.43
1:C:63:TRP:O	1:C:264:SER:N	2.44	0.43
1:C:341:TRP:HZ3	1:C:342:TYR:CE1	2.35	0.43
1:C:376:GLU:O	1:C:380:LYS:HG3	2.17	0.43
1:D:29:GLU:CD	1:D:35:LYS:HA	2.43	0.43
1:D:418:PHE:CD1	1:D:418:PHE:O	2.71	0.43
1:C:274:LYS:O	1:C:278:LYS:HG3	2.18	0.43
1:D:29:GLU:OE2	1:D:36:VAL:O	2.37	0.43
1:D:154:GLU:HG3	1:D:155:PRO:HD2	2.00	0.43
1:D:400:GLU:O	1:D:404:GLN:OE1	2.36	0.43
1:A:373:LYS:O	1:A:377:GLN:HG2	2.18	0.43
1:C:422:MET:HE3	1:C:422:MET:HB2	1.71	0.43
1:A:47:LYS:O	1:A:51:VAL:HG22	2.18	0.43
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.53	0.43
1:B:8:LEU:HD12	1:B:59:ASP:HB2	1.92	0.43
1:C:11:TRP:HB3	1:C:44:LEU:HD12	1.99	0.43
1:C:63:TRP:HD1	1:C:64:ALA:O	2.02	0.43
1:C:205:MET:HE3	1:C:205:MET:HB2	1.81	0.43
1:C:298:LYS:HZ2	1:C:300:LEU:HD23	1.82	0.43
1:D:15:ASP:CG	1:D:16:LYS:HZ1	2.27	0.43
1:D:274:LYS:O	1:D:278:LYS:HG3	2.18	0.43
1:B:48:PHE:CA	1:B:51:VAL:HG12	2.45	0.43
1:B:130:TRP:CD1	1:B:249:PRO:HB2	2.54	0.43
1:C:90:LEU:CD2	1:C:304:ALA:C	2.91	0.43
1:C:377:GLN:HA	1:C:380:LYS:HG3	2.00	0.43
1:A:101:ASN:C	1:A:103:LYS:HZ3	2.26	0.43
1:A:106:ALA:HB1	1:A:265:ALA:C	2.43	0.43
1:A:382:VAL:HG12	1:B:378:LEU:HD13	2.00	0.43
1:B:90:LEU:HD23	1:B:304:ALA:CB	2.49	0.43
1:C:90:LEU:CB	1:C:95:TRP:CZ2	2.95	0.43
1:C:303:VAL:HG22	1:C:309:GLU:OE1	2.19	0.43
1:C:314:LYS:HD3	1:C:314:LYS:C	2.43	0.43
1:A:111:VAL:N	1:A:302:ALA:O	2.41	0.43
1:D:26:LYS:O	1:D:26:LYS:HG2	2.19	0.43
1:D:138:LYS:HD2	1:D:138:LYS:HA	1.61	0.43
1:A:207:ALA:O	1:D:397:LYS:NZ	2.51	0.43
1:B:7:LYS:HB2	1:B:35:LYS:O	2.19	0.43
1:B:133:ILE:HG13	1:B:134:PRO:HD3	2.01	0.43
1:C:92:PRO:CD	1:C:306:LYS:HZ3	2.30	0.43
1:D:336:GLN:O	1:D:338:SER:N	2.51	0.43
1:B:86:PHE:HA	1:B:89:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:TYR:HD1	1:D:19:ASN:N	2.14	0.42
1:D:29:GLU:OE1	1:D:35:LYS:HA	2.19	0.42
1:D:435:LEU:HD12	1:D:435:LEU:N	2.34	0.42
1:A:7:LYS:HD2	1:A:35:LYS:CG	2.48	0.42
1:B:64:ALA:HB1	1:B:66:ASP:OD1	2.19	0.42
1:B:267:ILE:HD11	1:B:281:LEU:HD12	2.01	0.42
1:A:65:HIS:HB3	1:A:262:VAL:HG22	2.00	0.42
1:A:106:ALA:CA	1:A:265:ALA:O	2.67	0.42
1:B:21:LEU:HA	1:B:24:VAL:CG1	2.48	0.42
1:B:100:TYR:HB2	1:B:105:ILE:HG21	2.02	0.42
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.94	0.42
1:D:333:ASN:OD1	1:D:333:ASN:N	2.45	0.42
1:A:59:ASP:O	1:A:267:ILE:HA	2.19	0.42
1:A:98:VAL:HG21	1:A:106:ALA:HB3	2.01	0.42
1:A:278:LYS:O	1:A:282:GLU:HB2	2.19	0.42
1:C:246:THR:OG1	1:C:247:VAL:N	2.51	0.42
1:D:142:ALA:O	1:D:144:GLY:N	2.52	0.42
1:B:193:LEU:O	1:B:197:VAL:HG13	2.19	0.42
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.71	0.42
1:C:106:ALA:CB	1:C:265:ALA:C	2.87	0.42
1:A:21:LEU:HA	1:A:24:VAL:CG2	2.50	0.42
1:A:78:ALA:HB2	1:A:269:ALA:HA	2.01	0.42
1:A:278:LYS:O	1:A:282:GLU:CB	2.67	0.42
1:C:98:VAL:O	1:C:105:ILE:CG2	2.66	0.42
1:D:47:LYS:C	1:D:49:PRO:CD	2.88	0.42
1:D:147:ALA:O	1:D:225:MET:HG2	2.19	0.42
1:A:80:ILE:HD11	1:A:105:ILE:O	2.20	0.42
1:B:147:ALA:O	1:B:225:MET:N	2.53	0.42
1:B:281:LEU:HA	1:B:285:LEU:HB3	2.00	0.42
1:A:63:TRP:HB3	1:A:68:PHE:CE1	2.54	0.42
1:B:8:LEU:HD11	1:B:59:ASP:CG	2.44	0.42
1:C:62:PHE:HZ	1:C:285:LEU:CD2	2.33	0.42
1:D:80:ILE:O	1:D:82:PRO:HD3	2.20	0.42
1:D:105:ILE:H	1:D:105:ILE:HG13	1.71	0.42
1:A:129:THR:OG1	1:A:131:GLU:OE1	2.38	0.42
1:B:435:LEU:O	1:B:439:PHE:HB2	2.19	0.42
1:D:151:ASN:OD1	1:D:210:ASP:HA	2.20	0.42
1:A:305:LEU:HD23	1:A:306:LYS:N	2.35	0.41
1:B:12:ILE:O	1:B:40:HIS:HA	2.19	0.41
1:B:128:LYS:O	1:B:250:THR:HG22	2.20	0.41
1:A:267:ILE:HG12	1:A:277:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLU:HB2	1:A:401:GLU:HG3	2.01	0.41
1:B:110:ALA:HB1	1:B:302:ALA:O	2.21	0.41
1:B:110:ALA:CA	1:B:303:VAL:HA	2.46	0.41
1:B:155:PRO:HG3	1:B:345:ARG:HB2	2.01	0.41
1:B:355:ARG:HH21	1:C:397:LYS:NZ	2.18	0.41
1:C:76:LEU:O	1:C:77:LEU:HD12	2.19	0.41
1:C:90:LEU:CD2	1:C:305:LEU:HA	2.49	0.41
1:D:230:PRO:HA	1:D:233:TRP:CD2	2.54	0.41
1:A:108:PRO:O	1:A:286:LEU:HD21	2.20	0.41
1:B:12:ILE:CG2	1:B:13:ASN:H	2.32	0.41
1:C:12:ILE:O	1:C:40:HIS:HA	2.20	0.41
1:C:40:HIS:O	1:C:40:HIS:CG	2.72	0.41
1:D:45:GLU:O	1:D:45:GLU:HG3	2.21	0.41
1:D:73:GLN:HB2	1:D:100:TYR:OH	2.21	0.41
1:A:147:ALA:O	1:A:225:MET:N	2.54	0.41
1:B:79:GLU:CG	1:B:103:LYS:HB3	2.44	0.41
1:D:292:GLU:O	1:D:295:ASN:N	2.52	0.41
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.95	0.41
1:C:153:GLN:HB3	1:C:345:ARG:HH12	1.85	0.41
1:D:12:ILE:HD12	1:D:62:PHE:HB2	2.02	0.41
1:B:59:ASP:OD1	1:B:271:SER:HA	2.20	0.41
1:B:80:ILE:CD1	1:B:107:TYR:CE1	2.93	0.41
1:C:63:TRP:O	1:C:264:SER:OG	2.34	0.41
1:D:65:HIS:O	1:D:66:ASP:C	2.63	0.41
1:D:97:ALA:HA	1:D:330:ILE:HG21	2.02	0.41
1:B:116:LEU:HD22	1:B:249:PRO:HD3	2.02	0.41
1:B:118:TYR:CE1	1:B:126:PRO:HG3	2.56	0.41
1:C:50:GLN:HG3	1:C:423:LYS:HE3	2.02	0.41
1:C:391:VAL:HG12	1:C:403:LYS:HG3	2.03	0.41
1:D:80:ILE:HD11	1:D:267:ILE:HG12	2.02	0.41
1:D:96:ASP:OD1	1:D:96:ASP:N	2.52	0.41
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.21	0.41
1:D:153:GLN:HG3	1:D:210:ASP:HB3	2.03	0.41
1:D:377:GLN:HE22	1:D:380:LYS:CE	2.34	0.41
1:A:305:LEU:HD23	1:A:307:SER:N	2.36	0.41
1:B:3:ILE:HB	1:B:56:ASP:HA	2.03	0.41
1:B:179:ILE:C	1:B:181:ASP:H	2.28	0.41
1:C:4:GLU:OE1	1:C:7:LYS:N	2.44	0.41
1:D:179:ILE:HB	1:D:334:ILE:CD1	2.37	0.41
1:A:389:LYS:HE2	1:B:371:ASP:OD1	2.20	0.41
1:B:110:ALA:HB2	1:B:303:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ILE:H	1:C:3:ILE:HG13	1.68	0.41
1:C:63:TRP:CD1	1:C:64:ALA:HB3	2.56	0.41
1:C:81:THR:HG22	1:C:278:LYS:NZ	2.36	0.41
1:C:91:TYR:CB	1:C:94:THR:CG2	2.87	0.41
1:C:134:PRO:HG3	1:C:199:LEU:HD21	2.03	0.41
1:C:424:LYS:HD2	1:C:425:LYS:CB	2.42	0.41
1:D:17:GLY:HA3	1:D:294:VAL:HG23	2.03	0.41
1:D:46:GLU:CG	1:D:416:TRP:HH2	2.34	0.41
1:D:294:VAL:HG13	1:D:300:LEU:HD11	2.03	0.41
1:D:331:MET:HG3	1:D:332:PRO:CD	2.40	0.41
1:D:414:LYS:HE2	1:D:414:LYS:HB2	1.71	0.41
1:A:246:THR:OG1	1:A:247:VAL:N	2.53	0.41
1:A:394:ASN:ND2	1:A:398:LEU:O	2.54	0.41
1:B:104:LEU:HD13	1:B:104:LEU:HA	1.94	0.41
1:C:298:LYS:HZ2	1:C:298:LYS:HG3	1.64	0.41
1:D:343:ALA:HB2	1:D:369:ALA:HB2	2.02	0.41
1:C:315:ASP:OD2	1:C:317:ARG:NH1	2.54	0.40
1:C:372:LEU:HD23	1:C:372:LEU:HA	1.92	0.40
1:D:24:VAL:C	1:D:26:LYS:N	2.79	0.40
1:D:71:TYR:HA	1:D:76:LEU:HD23	2.03	0.40
1:A:309:GLU:O	1:A:313:ALA:N	2.49	0.40
1:B:28:PHE:O	1:B:32:THR:HG22	2.21	0.40
1:B:130:TRP:O	1:B:133:ILE:HG12	2.21	0.40
1:C:268:ASN:OD1	1:C:269:ALA:N	2.53	0.40
1:B:7:LYS:HE3	1:B:37:THR:HG23	2.03	0.40
1:B:107:TYR:O	1:B:264:SER:HA	2.21	0.40
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.57	0.40
1:B:280:PHE:O	1:B:284:TYR:HB2	2.20	0.40
1:D:47:LYS:H	1:D:49:PRO:HD3	1.85	0.40
1:A:364:ALA:O	1:A:368:ASN:HB2	2.21	0.40
1:B:13:ASN:CG	1:B:14:GLY:N	2.78	0.40
1:B:246:THR:OG1	1:B:247:VAL:N	2.55	0.40
1:C:130:TRP:HB3	1:C:195:PHE:CE2	2.56	0.40
1:C:155:PRO:HD2	1:C:341:TRP:CZ2	2.55	0.40
1:D:30:LYS:HE2	1:D:30:LYS:HA	2.04	0.40
1:D:112:GLU:N	1:D:261:GLY:O	2.52	0.40
1:D:190:LYS:HD2	1:D:359:ASP:OD1	2.21	0.40
1:D:314:LYS:HE2	1:D:314:LYS:HB3	1.92	0.40
1:A:178:ASP:HB3	1:A:181:ASP:HB3	2.02	0.40
1:D:388:GLU:O	1:D:391:VAL:HG22	2.21	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	423/462 (92%)	393 (93%)	26 (6%)	4 (1%)	14	41
1	B	393/462 (85%)	357 (91%)	32 (8%)	4 (1%)	12	38
1	C	411/462 (89%)	389 (95%)	19 (5%)	3 (1%)	18	47
1	D	409/462 (88%)	365 (89%)	36 (9%)	8 (2%)	6	21
All	All	1636/1848 (88%)	1504 (92%)	113 (7%)	19 (1%)	10	34

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
1	A	399	LYS
1	A	400	GLU
1	B	335	PRO
1	C	241	VAL
1	D	334	ILE
1	D	436	GLN
1	A	33	GLY
1	B	75	GLY
1	B	101	ASN
1	C	42	ASP
1	D	435	LEU
1	D	143	LYS
1	D	411	ARG
1	B	336	GLN
1	D	434	LEU
1	D	337	MET
1	C	88	ASP
1	D	48	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	342/373 (92%)	329 (96%)	13 (4%)	29	64
1	B	318/373 (85%)	299 (94%)	19 (6%)	17	47
1	C	338/373 (91%)	328 (97%)	10 (3%)	36	72
1	D	333/373 (89%)	312 (94%)	21 (6%)	16	45
All	All	1331/1492 (89%)	1268 (95%)	63 (5%)	23	57

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	31	ASP
1	A	256	SER
1	A	257	LYS
1	A	275	GLU
1	A	276	LEU
1	A	278	LYS
1	A	282	GLU
1	A	285	LEU
1	A	287	THR
1	A	399	LYS
1	A	400	GLU
1	A	401	GLU
1	B	8	LEU
1	B	10	ILE
1	B	12	ILE
1	B	61	ILE
1	B	63	TRP
1	B	65	HIS
1	B	66	ASP
1	B	67	ARG
1	B	68	PHE
1	B	76	LEU
1	B	89	LYS

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Mol	Chain	Res	Type
1	B	99	ARG
1	B	103	LYS
1	B	273	ASN
1	B	274	LYS
1	B	305	LEU
1	B	334	ILE
1	B	441	VAL
1	B	442	ASP
1	C	42	ASP
1	C	44	LEU
1	C	68	PHE
1	C	88	ASP
1	C	90	LEU
1	C	94	THR
1	C	105	ILE
1	C	292	GLU
1	C	336	GLN
1	C	422	MET
1	D	24	VAL
1	D	48	PHE
1	D	50	GLN
1	D	51	VAL
1	D	139	GLU
1	D	141	LYS
1	D	171	LYS
1	D	172	TYR
1	D	179	ILE
1	D	310	GLU
1	D	311	GLU
1	D	331	MET
1	D	333	ASN
1	D	334	ILE
1	D	336	GLN
1	D	337	MET
1	D	359	ASP
1	D	422	MET
1	D	432	GLU
1	D	433	MET
1	D	434	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	333	ASN
1	A	356	GLN
1	B	65	HIS
1	B	326	GLN
1	B	333	ASN
1	B	356	GLN
1	C	65	HIS
1	C	73	GLN
1	C	356	GLN
1	C	377	GLN
1	D	50	GLN
1	D	204	HIS
1	D	228	ASN
1	D	283	ASN
1	D	377	GLN
1	D	408	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	427/462 (92%)	1.06	62 (14%) 6 4	54, 108, 184, 260	0
1	B	399/462 (86%)	1.24	88 (22%) 2 2	58, 114, 222, 270	0
1	C	419/462 (90%)	1.22	78 (18%) 3 2	58, 116, 221, 264	0
1	D	415/462 (89%)	1.25	73 (17%) 4 3	60, 115, 222, 331	0
All	All	1660/1848 (89%)	1.19	301 (18%) 3 3	54, 114, 220, 331	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	GLY	5.8
1	D	119	ASN	5.7
1	B	183	GLY	5.6
1	C	66	ASP	5.6
1	C	17	GLY	5.3
1	D	223	THR	5.1
1	C	95	TRP	5.0
1	B	164	ALA	4.8
1	B	439	PHE	4.7
1	D	221	GLY	4.6
1	C	137	ASP	4.5
1	C	241	VAL	4.5
1	D	416	TRP	4.4
1	D	58	PRO	4.4
1	A	76	LEU	4.3
1	B	64	ALA	4.0
1	B	240	ALA	4.0
1	C	336	GLN	3.9
1	C	312	LEU	3.9
1	D	224	ALA	3.9
1	A	291	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	177	TYR	3.8
1	C	57	GLY	3.8
1	B	83	ALA	3.8
1	C	221	GLY	3.8
1	C	313	ALA	3.7
1	B	104	LEU	3.7
1	C	343	ALA	3.7
1	D	209	THR	3.6
1	A	77	LEU	3.6
1	C	338	SER	3.6
1	C	198	ASP	3.6
1	A	184	VAL	3.6
1	B	18	TYR	3.6
1	C	58	PRO	3.6
1	D	293	ALA	3.5
1	B	13	ASN	3.5
1	D	199	LEU	3.5
1	B	165	ASP	3.5
1	B	16	LYS	3.5
1	B	110	ALA	3.5
1	A	276	LEU	3.5
1	A	367	THR	3.5
1	B	37	THR	3.5
1	D	20	GLY	3.5
1	C	89	LYS	3.5
1	A	277	ALA	3.4
1	D	337	MET	3.4
1	D	51	VAL	3.4
1	A	90	LEU	3.4
1	B	77	LEU	3.4
1	D	241	VAL	3.3
1	D	80	ILE	3.3
1	A	98	VAL	3.3
1	D	133	ILE	3.3
1	C	146	SER	3.3
1	C	302	ALA	3.2
1	D	142	ALA	3.2
1	A	8	LEU	3.2
1	C	140	LEU	3.2
1	B	82	PRO	3.2
1	A	421	ALA	3.2
1	D	64	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	174	ALA	3.2
1	B	184	VAL	3.2
1	B	167	GLY	3.2
1	B	68	PHE	3.1
1	B	24	VAL	3.1
1	A	332	PRO	3.1
1	B	263	LEU	3.1
1	D	118	TYR	3.1
1	D	372	LEU	3.1
1	D	68	PHE	3.1
1	A	125	ASN	3.1
1	A	350	ASN	3.1
1	A	287	THR	3.1
1	B	32	THR	3.1
1	C	339	ALA	3.0
1	D	277	ALA	3.0
1	D	291	LEU	3.0
1	B	93	PHE	3.0
1	A	57	GLY	3.0
1	B	267	ILE	3.0
1	A	390	LEU	3.0
1	A	126	PRO	3.0
1	D	82	PRO	3.0
1	D	28	PHE	3.0
1	A	334	ILE	3.0
1	C	59	ASP	3.0
1	A	124	PRO	3.0
1	B	443	PRO	3.0
1	C	86	PHE	3.0
1	C	90	LEU	3.0
1	C	420	ASP	3.0
1	B	106	ALA	3.0
1	A	30	LYS	2.9
1	D	226	THR	2.9
1	D	220	LYS	2.9
1	A	273	ASN	2.9
1	D	208	ASP	2.9
1	C	291	LEU	2.9
1	B	199	LEU	2.9
1	D	140	LEU	2.9
1	B	17	GLY	2.9
1	B	339	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	100	TYR	2.8
1	B	91	TYR	2.8
1	B	382	VAL	2.8
1	C	184	VAL	2.8
1	D	371	ASP	2.8
1	C	104	LEU	2.8
1	D	44	LEU	2.8
1	D	300	LEU	2.8
1	D	149	MET	2.8
1	B	129	THR	2.8
1	A	183	GLY	2.8
1	D	41	PRO	2.8
1	C	358	VAL	2.8
1	C	430	VAL	2.8
1	D	36	VAL	2.8
1	C	61	ILE	2.8
1	D	283	ASN	2.8
1	B	66	ASP	2.8
1	C	346	THR	2.8
1	D	335	PRO	2.8
1	B	179	ILE	2.7
1	B	276	LEU	2.7
1	A	274	LYS	2.7
1	B	75	GLY	2.7
1	A	85	ALA	2.7
1	B	8	LEU	2.7
1	C	76	LEU	2.7
1	C	398	LEU	2.7
1	D	83	ALA	2.7
1	D	207	ALA	2.7
1	C	324	ASN	2.7
1	D	32	THR	2.7
1	A	82	PRO	2.7
1	C	309	GLU	2.7
1	C	182	VAL	2.7
1	A	164	ALA	2.7
1	B	369	ALA	2.7
1	D	34	ILE	2.7
1	B	65	HIS	2.7
1	B	6	GLY	2.7
1	B	48	PHE	2.7
1	D	63	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	286	LEU	2.7
1	A	169	ALA	2.6
1	B	185	ASP	2.6
1	A	267	ILE	2.6
1	B	74	SER	2.6
1	D	48	PHE	2.6
1	B	286	LEU	2.6
1	B	304	ALA	2.6
1	B	49	PRO	2.6
1	A	333	ASN	2.6
1	D	225	MET	2.6
1	A	438	PHE	2.6
1	B	28	PHE	2.6
1	C	68	PHE	2.6
1	D	53	ALA	2.6
1	D	239	SER	2.6
1	B	431	GLY	2.6
1	C	136	LEU	2.6
1	A	29	GLU	2.5
1	A	78	ALA	2.5
1	B	182	VAL	2.5
1	B	302	ALA	2.5
1	A	80	ILE	2.5
1	A	36	VAL	2.5
1	C	391	VAL	2.5
1	C	416	TRP	2.5
1	B	71	TYR	2.5
1	B	168	TYR	2.5
1	D	369	ALA	2.5
1	A	208	ASP	2.5
1	B	31	ASP	2.5
1	C	62	PHE	2.5
1	B	10	ILE	2.4
1	B	440	SER	2.4
1	C	98	VAL	2.4
1	B	387	LEU	2.4
1	B	63	TRP	2.4
1	C	340	PHE	2.4
1	D	84	ALA	2.4
1	A	437	THR	2.4
1	D	200	ILE	2.4
1	C	276	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	105	ILE	2.4
1	A	283	ASN	2.4
1	D	344	VAL	2.4
1	C	220	LYS	2.4
1	A	97	ALA	2.4
1	C	421	ALA	2.4
1	C	71	TYR	2.4
1	C	263	LEU	2.4
1	B	51	VAL	2.3
1	C	395	VAL	2.3
1	B	266	GLY	2.3
1	A	281	LEU	2.3
1	C	305	LEU	2.3
1	A	60	ILE	2.3
1	D	38	VAL	2.3
1	A	175	GLY	2.3
1	D	273	ASN	2.3
1	B	78	ALA	2.3
1	B	169	ALA	2.3
1	B	311	GLU	2.3
1	D	243	TYR	2.3
1	D	370	VAL	2.3
1	B	166	GLY	2.3
1	D	290	GLY	2.3
1	C	72	ALA	2.3
1	B	15	ASP	2.3
1	C	11	TRP	2.3
1	D	117	ILE	2.3
1	D	146	SER	2.3
1	D	339	ALA	2.3
1	C	77	LEU	2.3
1	C	297	ASP	2.3
1	B	95	TRP	2.3
1	C	341	TRP	2.3
1	B	441	VAL	2.3
1	C	258	PRO	2.3
1	C	253	GLY	2.3
1	A	187	ALA	2.2
1	C	21	LEU	2.2
1	D	414	LYS	2.2
1	C	88	ASP	2.2
1	D	198	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	433	MET	2.2
1	C	433	MET	2.2
1	C	370	VAL	2.2
1	B	20	GLY	2.2
1	C	354	GLY	2.2
1	C	331	MET	2.2
1	B	163	ALA	2.2
1	B	172	TYR	2.2
1	B	161	LEU	2.2
1	B	390	LEU	2.2
1	C	83	ALA	2.2
1	D	72	ALA	2.2
1	C	350	ASN	2.2
1	B	40	HIS	2.2
1	B	9	VAL	2.2
1	A	435	LEU	2.2
1	B	329	GLU	2.2
1	B	273	ASN	2.1
1	A	127	PRO	2.1
1	C	36	VAL	2.1
1	D	210	ASP	2.1
1	C	183	GLY	2.1
1	D	238	THR	2.1
1	B	97	ALA	2.1
1	C	356	GLN	2.1
1	D	13	ASN	2.1
1	A	38	VAL	2.1
1	B	391	VAL	2.1
1	A	32	THR	2.1
1	B	94	THR	2.1
1	C	123	LEU	2.1
1	B	365	ALA	2.1
1	C	342	TYR	2.1
1	D	222	GLU	2.1
1	A	382	VAL	2.1
1	B	272	PRO	2.1
1	C	134	PRO	2.1
1	C	219	ASN	2.1
1	C	185	ASP	2.1
1	D	75	GLY	2.1
1	C	318	ILE	2.1
1	B	98	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	314	LYS	2.1
1	B	44	LEU	2.1
1	D	70	GLY	2.1
1	A	165	ASP	2.1
1	C	226	THR	2.1
1	A	341	TRP	2.1
1	B	109	ILE	2.1
1	D	147	ALA	2.1
1	B	5	GLU	2.1
1	D	310	GLU	2.1
1	C	73	GLN	2.0
1	C	51	VAL	2.0
1	C	286	LEU	2.0
1	A	102	GLY	2.0
1	A	166	GLY	2.0
1	D	438	PHE	2.0
1	A	209	THR	2.0
1	C	191	ALA	2.0
1	D	413	ASP	2.0
1	B	11	TRP	2.0
1	D	274	LYS	2.0
1	A	338	SER	2.0
1	A	160	PRO	2.0
1	B	76	LEU	2.0
1	A	266	GLY	2.0
1	A	83	ALA	2.0
1	B	367	THR	2.0
1	B	294	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.