



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:45 AM EDT

PDB ID : 1VCW / pdb_00001vcw
Title : Crystal structure of DegS after backsoaking the activating peptide
Authors : Wilken, C.; Kitzing, K.; Kurzbauer, R.; Ehrmann, M.; Clausen, T.
Deposited on : 2004-03-16
Resolution : 3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

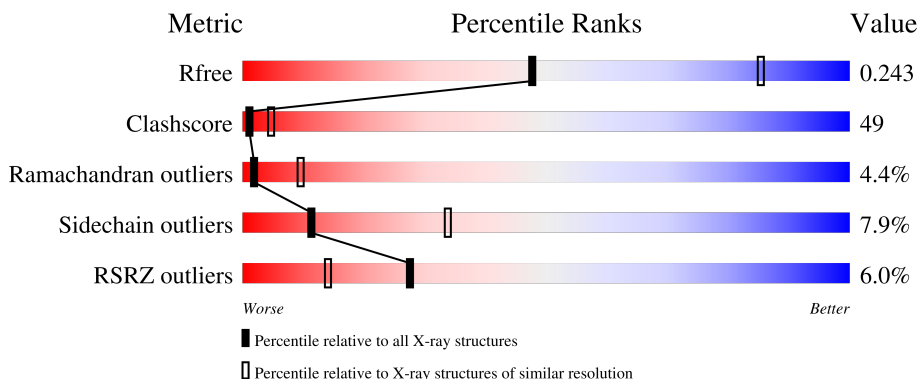
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	314	4% 39% 42% 10% 7%
1	B	314	4% 38% 45% 8% 7%
1	C	314	8% 38% 45% 9% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6384 atoms, of which 0 are hydrogens and 0 are deuteriums.

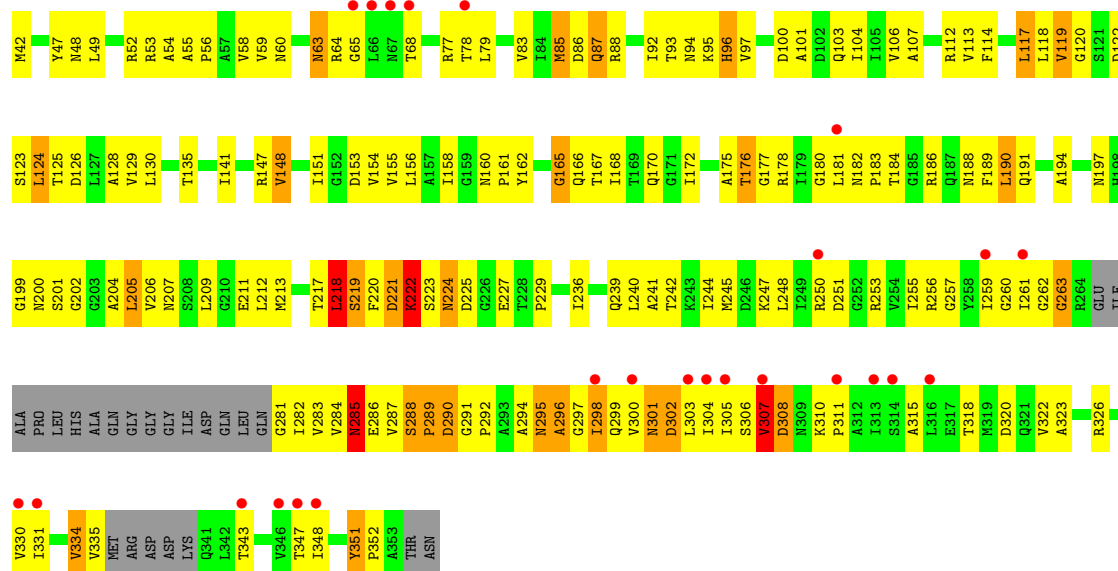
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protease degS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2128	1329	380	414	5			
1	B	291	Total	C	N	O	S	51	0	0
			2128	1329	380	414	5			
1	C	291	Total	C	N	O	S	0	0	0
			2128	1329	380	414	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	initiating methionine	UNP P31137
B	42	MET	-	initiating methionine	UNP P31137
C	42	MET	-	initiating methionine	UNP P31137



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.99Å 142.73Å 41.23Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 20.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.05) 96.1 (20.00-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.04Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.301 0.243 , 0.243	Depositor DCC
R_{free} test set	1106 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6384	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 4.47% 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	0.84	5/2155 (0.2%)	1.31	28/2935 (1.0%)
1	B	1.08	5/2155 (0.2%)	1.47	35/2935 (1.2%)
1	C	0.70	3/2155 (0.1%)	1.33	34/2935 (1.2%)
All	All	0.89	13/6465 (0.2%)	1.37	97/8805 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	ASN	C-N	-35.22	0.88	1.33
1	A	219	SER	N-CA	-9.21	1.35	1.45
1	B	227	GLU	C-N	8.23	1.59	1.33
1	A	260	GLY	C-N	7.91	1.38	1.33
1	C	334	VAL	N-CA	7.79	1.56	1.46
1	A	220	PHE	N-CA	-7.10	1.37	1.46
1	B	217	THR	CA-C	-6.59	1.45	1.52
1	A	219	SER	C-N	-5.92	1.25	1.33
1	B	289	PRO	N-CA	-5.92	1.39	1.47
1	C	223	SER	N-CA	5.55	1.53	1.46
1	C	222	LYS	N-CA	5.20	1.52	1.46
1	B	334	VAL	N-CA	5.01	1.52	1.46
1	A	259	ILE	CA-C	-5.01	1.46	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ASN	O-C-N	-26.83	86.90	122.59
1	B	224	ASN	CA-C-N	-13.73	100.16	121.86
1	B	224	ASN	C-N-CA	-13.73	100.16	121.86
1	C	334	VAL	CB-CA-C	-13.53	89.10	111.29
1	B	334	VAL	CB-CA-C	-13.08	89.84	111.29
1	B	289	PRO	N-CA-C	-12.44	93.54	111.33
1	B	219	SER	CA-C-N	10.54	141.66	121.54
1	B	219	SER	C-N-CA	10.54	141.66	121.54
1	C	288	SER	CA-C-N	-10.49	108.96	119.76
1	C	288	SER	C-N-CA	-10.49	108.96	119.76
1	B	299	GLN	OE1-CD-NE2	-10.32	112.28	122.60
1	A	299	GLN	OE1-CD-NE2	-10.07	112.53	122.60
1	B	217	THR	CB-CA-C	-9.76	98.45	110.94
1	C	299	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	B	225	ASP	CA-CB-CG	-9.54	103.06	112.60
1	B	307	VAL	N-CA-C	-9.03	98.01	109.30
1	A	259	ILE	N-CA-C	-8.61	91.43	109.34
1	A	307	VAL	N-CA-C	-8.55	97.56	108.84
1	B	219	SER	CA-C-O	8.23	129.11	120.30
1	A	226	GLY	N-CA-C	-8.18	103.13	114.67
1	A	259	ILE	CB-CA-C	-8.05	98.09	111.29
1	A	260	GLY	CA-C-N	8.04	130.01	121.97
1	A	260	GLY	C-N-CA	8.04	130.01	121.97
1	B	85	MET	N-CA-C	7.73	119.78	111.36
1	C	218	LEU	CA-C-N	7.66	131.75	120.87
1	C	218	LEU	C-N-CA	7.66	131.75	120.87
1	C	307	VAL	N-CA-C	-7.50	99.24	109.37
1	C	285	ASN	CB-CA-C	-7.47	98.48	110.81
1	B	220	PHE	N-CA-CB	-7.39	98.01	110.49
1	C	289	PRO	CA-N-CD	-7.38	101.67	112.00
1	B	299	GLN	CG-CD-NE2	7.15	127.13	116.40
1	C	222	LYS	CA-C-N	7.11	135.13	121.54
1	C	222	LYS	C-N-CA	7.11	135.13	121.54
1	B	219	SER	O-C-N	7.10	131.50	123.27
1	A	85	MET	N-CA-C	7.01	120.31	111.69
1	B	135	THR	N-CA-C	-7.01	98.89	110.17
1	A	258	TYR	CA-C-N	6.98	134.54	121.97
1	A	258	TYR	C-N-CA	6.98	134.54	121.97
1	C	85	MET	N-CA-C	6.98	119.91	111.82
1	A	223	SER	N-CA-C	-6.92	106.03	114.75
1	C	299	GLN	CG-CD-NE2	6.58	126.27	116.40
1	C	218	LEU	O-C-N	6.57	131.32	122.59
1	C	334	VAL	N-CA-C	6.49	122.84	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	SER	N-CA-C	-6.49	100.68	110.28
1	A	241	ALA	N-CA-C	-6.39	104.32	111.28
1	B	165	GLY	N-CA-C	-6.38	104.61	112.33
1	C	289	PRO	N-CA-C	-6.32	101.27	111.14
1	B	307	VAL	N-CA-CB	6.31	118.07	110.31
1	B	115	GLU	N-CA-C	-6.30	99.38	109.96
1	C	220	PHE	CB-CA-C	6.24	119.62	110.26
1	B	220	PHE	N-CA-C	6.23	124.06	110.80
1	A	190	LEU	N-CA-C	-6.18	99.64	109.59
1	B	217	THR	N-CA-CB	6.18	119.39	110.37
1	A	289	PRO	N-CA-C	-6.09	99.91	112.47
1	A	299	GLN	CG-CD-NE2	6.06	125.49	116.40
1	B	307	VAL	CB-CA-C	-6.03	102.34	111.33
1	C	307	VAL	N-CA-CB	6.02	118.20	110.13
1	B	298	ILE	N-CA-C	6.00	121.81	109.34
1	A	307	VAL	N-CA-CB	5.95	117.43	110.82
1	A	290	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	298	ILE	CA-C-N	5.92	133.34	122.92
1	A	298	ILE	C-N-CA	5.92	133.34	122.92
1	A	292	PRO	CA-N-CD	-5.88	103.77	112.00
1	B	334	VAL	N-CA-C	5.88	121.56	109.34
1	B	205	LEU	N-CA-C	-5.73	97.82	108.02
1	A	135	THR	N-CA-C	-5.72	100.86	109.95
1	B	263	GLY	N-CA-C	5.64	117.51	110.29
1	C	241	ALA	N-CA-C	-5.62	105.15	111.28
1	C	165	GLY	N-CA-C	-5.61	106.01	112.29
1	B	194	ALA	N-CA-C	-5.61	102.60	110.50
1	A	298	ILE	N-CA-C	5.58	120.94	109.34
1	C	88	ARG	N-CA-C	-5.56	106.00	112.89
1	B	134	ALA	N-CA-C	5.55	117.77	108.73
1	B	190	LEU	N-CA-C	-5.55	100.66	109.59
1	C	221	ASP	CA-CB-CG	-5.53	107.07	112.60
1	B	45	ALA	N-CA-C	-5.44	102.34	110.23
1	C	148	VAL	CA-C-N	5.40	125.33	119.76
1	C	148	VAL	C-N-CA	5.40	125.33	119.76
1	B	295	ASN	CA-C-N	-5.38	111.27	121.54
1	B	295	ASN	C-N-CA	-5.38	111.27	121.54
1	A	165	GLY	N-CA-C	-5.37	104.65	112.17
1	A	263	GLY	N-CA-C	5.37	116.98	111.56
1	A	219	SER	O-C-N	5.32	129.01	122.84
1	C	222	LYS	N-CA-C	5.31	122.11	110.80
1	C	194	ALA	N-CA-C	-5.20	102.58	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	GLY	N-CA-C	5.18	117.04	110.20
1	C	87	GLN	N-CA-C	5.18	119.36	113.19
1	B	227	GLU	O-C-N	5.17	129.47	122.59
1	A	132	ILE	N-CA-C	-5.12	101.29	109.17
1	C	190	LEU	N-CA-C	-5.09	101.40	109.59
1	A	218	LEU	O-C-N	5.08	128.03	123.26
1	B	130	LEU	N-CA-C	-5.08	102.64	109.95
1	C	307	VAL	CB-CA-C	-5.07	103.32	111.59
1	A	286	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	176	THR	N-CA-C	5.02	119.27	112.04
1	C	220	PHE	CA-CB-CG	-5.01	108.79	113.80
1	C	218	LEU	CA-C-O	5.01	127.67	120.51

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	224	ASN	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	2128	0	2124	216	5
1	B	2128	0	2125	217	4
1	C	2128	0	2127	215	1
All	All	6384	0	6376	623	5

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 49.

All (623) 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:218:LEU:HD13	1:B:219:SER:N	1.41	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PRO:HD3	1:A:349:GLN:OE1	1.32	1.30
1:C:218:LEU:HD13	1:C:218:LEU:O	1.18	1.27
1:C:334:VAL:O	1:C:335:VAL:CB	1.95	1.13
1:C:334:VAL:O	1:C:334:VAL:HG12	1.36	1.11
1:C:218:LEU:HD13	1:C:218:LEU:C	1.74	1.11
1:B:59:VAL:HG11	1:B:106:VAL:HG13	1.24	1.10
1:C:59:VAL:HG11	1:C:106:VAL:HG13	1.30	1.09
1:A:292:PRO:CD	1:A:349:GLN:OE1	2.00	1.08
1:C:218:LEU:HD22	1:C:219:SER:O	1.53	1.07
1:A:59:VAL:HG11	1:A:106:VAL:HG13	1.12	1.07
1:B:260:GLY:O	1:B:289:PRO:HG2	1.55	1.07
1:B:218:LEU:HD13	1:B:218:LEU:C	1.77	1.05
1:B:78:THR:HG22	1:B:79:LEU:H	1.18	1.05
1:B:147:ARG:HD2	1:B:211:GLU:OE2	1.55	1.04
1:B:226:GLY:O	1:B:227:GLU:HB3	1.51	1.04
1:C:147:ARG:HD2	1:C:211:GLU:OE2	1.57	1.04
1:C:218:LEU:O	1:C:218:LEU:CD1	2.06	1.02
1:B:334:VAL:O	1:B:335:VAL:CB	2.04	1.02
1:C:334:VAL:O	1:C:334:VAL:CG1	1.98	1.00
1:C:217:THR:O	1:C:218:LEU:HB3	1.61	0.99
1:B:334:VAL:O	1:B:334:VAL:HG12	1.61	0.99
1:A:295:ASN:O	1:A:296:ALA:HB2	1.59	0.98
1:B:218:LEU:HD23	1:B:233:GLY:HA2	1.45	0.98
1:B:218:LEU:C	1:B:218:LEU:CD1	2.35	0.97
1:B:260:GLY:C	1:B:289:PRO:HG2	1.90	0.96
1:A:292:PRO:HD3	1:A:349:GLN:CD	1.89	0.96
1:A:220:PHE:O	1:A:229:PRO:HG2	1.65	0.95
1:C:221:ASP:HB3	1:C:229:PRO:HG2	1.47	0.95
1:A:197:ASN:H	1:A:200:ASN:HD22	1.09	0.94
1:A:182:ASN:HD22	1:A:183:PRO:HD2	1.31	0.94
1:B:197:ASN:H	1:B:200:ASN:HD22	1.17	0.93
1:A:78:THR:HG22	1:A:79:LEU:H	1.34	0.92
1:A:147:ARG:HD2	1:A:211:GLU:OE2	1.68	0.92
1:A:290:ASP:O	1:A:291:GLY:O	1.87	0.92
1:A:259:ILE:O	1:A:259:ILE:CG2	2.17	0.91
1:C:59:VAL:HG13	1:C:107:ALA:O	1.71	0.90
1:C:78:THR:HG22	1:C:79:LEU:H	1.34	0.90
1:C:221:ASP:HB3	1:C:229:PRO:CG	2.02	0.90
1:B:308:ASP:OD2	1:B:331:ILE:CG2	2.21	0.89
1:C:197:ASN:H	1:C:200:ASN:HD22	1.17	0.89
1:C:182:ASN:HD22	1:C:183:PRO:HD2	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:CD2	1:C:219:SER:O	2.21	0.89
1:A:161:PRO:HA	1:A:199:GLY:HA3	1.56	0.88
1:B:59:VAL:HG13	1:B:107:ALA:O	1.73	0.88
1:A:330:VAL:HG22	1:A:347:THR:HG22	1.53	0.88
1:B:182:ASN:HD22	1:B:183:PRO:HD2	1.36	0.87
1:B:226:GLY:O	1:B:227:GLU:CB	2.22	0.87
1:A:259:ILE:O	1:A:259:ILE:HG23	1.74	0.87
1:A:63:ASN:C	1:A:63:ASN:HD22	1.81	0.87
1:B:63:ASN:C	1:B:63:ASN:HD22	1.82	0.87
1:C:330:VAL:HG22	1:C:347:THR:HG22	1.57	0.87
1:C:63:ASN:C	1:C:63:ASN:HD22	1.85	0.85
1:B:178:ARG:HH11	1:B:178:ARG:HB3	1.43	0.83
1:B:330:VAL:HG22	1:B:347:THR:HG22	1.57	0.83
1:A:259:ILE:HD11	1:A:261:ILE:HD12	1.58	0.83
1:B:118:LEU:HD23	1:B:120:GLY:H	1.43	0.83
1:C:178:ARG:HB3	1:C:178:ARG:NH1	1.94	0.83
1:A:197:ASN:H	1:A:200:ASN:ND2	1.77	0.82
1:C:125:THR:HG21	1:C:244:ILE:HD11	1.61	0.82
1:C:118:LEU:HD23	1:C:120:GLY:H	1.45	0.81
1:A:124:LEU:HD12	1:A:256:ARG:NH1	1.96	0.81
1:B:161:PRO:HA	1:B:199:GLY:HA3	1.63	0.80
1:B:334:VAL:O	1:B:334:VAL:CG1	2.15	0.80
1:B:217:THR:O	1:B:234:PHE:O	2.00	0.80
1:A:197:ASN:N	1:A:200:ASN:HD22	1.80	0.80
1:C:178:ARG:HB3	1:C:178:ARG:HH11	1.45	0.80
1:C:260:GLY:C	1:C:289:PRO:HG2	2.07	0.80
1:C:124:LEU:HD13	1:C:183:PRO:HG3	1.64	0.79
1:B:178:ARG:HB3	1:B:178:ARG:NH1	1.96	0.79
1:A:285:ASN:O	1:A:285:ASN:ND2	2.16	0.79
1:B:218:LEU:CD1	1:B:219:SER:N	2.36	0.79
1:C:253:ARG:NH1	1:C:255:ILE:HG12	1.98	0.79
1:A:182:ASN:HD22	1:A:183:PRO:CD	1.96	0.78
1:C:285:ASN:O	1:C:285:ASN:ND2	2.16	0.78
1:B:125:THR:HG21	1:B:244:ILE:CD1	2.14	0.78
1:A:59:VAL:CG1	1:A:106:VAL:HG13	2.05	0.78
1:B:308:ASP:OD2	1:B:331:ILE:HG21	1.83	0.78
1:C:295:ASN:O	1:C:296:ALA:HB2	1.83	0.77
1:A:178:ARG:HH11	1:A:178:ARG:HB3	1.50	0.77
1:C:222:LYS:HG2	1:C:224:ASN:O	1.85	0.77
1:C:260:GLY:O	1:C:289:PRO:HG2	1.84	0.77
1:B:253:ARG:NH1	1:B:255:ILE:HG12	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PRO:HA	1:C:199:GLY:HA3	1.67	0.76
1:A:178:ARG:HB3	1:A:178:ARG:NH1	2.00	0.76
1:A:222:LYS:HD2	1:B:162:TYR:CD2	2.18	0.76
1:A:255:ILE:HD12	1:A:326:ARG:HH12	1.50	0.76
1:C:129:VAL:HG23	1:C:248:LEU:HD12	1.67	0.76
1:A:260:GLY:C	1:A:289:PRO:HG2	2.10	0.76
1:A:125:THR:HG21	1:A:244:ILE:HD11	1.68	0.76
1:C:94:ASN:HA	1:C:126:ASP:O	1.85	0.75
1:A:59:VAL:HG11	1:A:106:VAL:CG1	2.06	0.75
1:B:78:THR:HG22	1:B:79:LEU:N	1.99	0.75
1:C:259:ILE:HD11	1:C:261:ILE:HD12	1.67	0.74
1:A:288:SER:N	1:A:289:PRO:HD3	2.03	0.74
1:A:118:LEU:HD23	1:A:120:GLY:H	1.51	0.74
1:A:295:ASN:O	1:A:296:ALA:CB	2.28	0.74
1:A:253:ARG:NH1	1:A:255:ILE:HG12	2.02	0.74
1:B:124:LEU:HD13	1:B:183:PRO:HG3	1.69	0.74
1:B:129:VAL:HG23	1:B:248:LEU:HD12	1.70	0.74
1:B:218:LEU:HD13	1:B:219:SER:CA	2.18	0.74
1:B:257:GLY:H	1:B:323:ALA:HA	1.53	0.73
1:B:207:ASN:HD22	1:B:213:MET:HE2	1.52	0.73
1:C:289:PRO:HD2	1:C:289:PRO:O	1.86	0.73
1:B:310:LYS:HG3	1:B:311:PRO:HD2	1.71	0.73
1:B:160:ASN:HD21	1:B:165:GLY:H	1.36	0.73
1:A:220:PHE:HD1	1:A:229:PRO:CB	2.01	0.73
1:B:295:ASN:O	1:B:296:ALA:HB2	1.88	0.73
1:C:197:ASN:H	1:C:200:ASN:ND2	1.87	0.73
1:B:197:ASN:H	1:B:200:ASN:ND2	1.88	0.72
1:B:94:ASN:HA	1:B:126:ASP:O	1.90	0.72
1:A:181:LEU:HD22	1:A:247:LYS:HE3	1.72	0.72
1:A:334:VAL:HG12	1:A:335:VAL:H	1.55	0.71
1:B:182:ASN:HD22	1:B:183:PRO:CD	2.03	0.71
1:A:59:VAL:HG13	1:A:107:ALA:O	1.89	0.71
1:A:191:GLN:HE22	1:B:167:THR:HG21	1.53	0.71
1:A:160:ASN:HD21	1:A:165:GLY:H	1.35	0.71
1:A:226:GLY:C	1:A:227:GLU:HG3	2.14	0.71
1:B:125:THR:HG21	1:B:244:ILE:HD11	1.73	0.71
1:C:182:ASN:HD22	1:C:183:PRO:CD	2.04	0.71
1:C:305:ILE:HB	1:C:334:VAL:HB	1.73	0.71
1:C:125:THR:HG21	1:C:244:ILE:CD1	2.21	0.70
1:A:94:ASN:HA	1:A:126:ASP:O	1.91	0.70
1:C:294:ALA:O	1:C:296:ALA:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLY:H	1:A:323:ALA:HA	1.56	0.70
1:A:177:GLY:HA3	1:A:189:PHE:O	1.92	0.70
1:B:191:GLN:HE22	1:C:167:THR:HG21	1.57	0.70
1:C:250:ARG:HH11	1:C:250:ARG:HB2	1.56	0.70
1:C:257:GLY:H	1:C:323:ALA:HA	1.55	0.70
1:B:288:SER:C	1:B:289:PRO:O	2.30	0.70
1:B:305:ILE:HB	1:B:334:VAL:HB	1.72	0.70
1:A:172:ILE:HG23	1:B:170:GLN:HG2	1.74	0.69
1:C:255:ILE:HD12	1:C:326:ARG:HH12	1.57	0.69
1:A:285:ASN:ND2	1:A:285:ASN:C	2.50	0.69
1:B:261:ILE:HG22	1:B:262:GLY:N	2.07	0.69
1:A:125:THR:HG21	1:A:244:ILE:CD1	2.24	0.68
1:C:310:LYS:HG3	1:C:311:PRO:HD2	1.74	0.68
1:A:170:GLN:HG2	1:C:172:ILE:HG23	1.74	0.68
1:B:155:VAL:HG22	1:B:205:LEU:HD22	1.76	0.68
1:A:225:ASP:CG	1:A:226:GLY:H	2.01	0.67
1:A:310:LYS:HG3	1:A:311:PRO:HD2	1.76	0.67
1:B:124:LEU:HD12	1:B:256:ARG:NH1	2.09	0.67
1:A:180:GLY:HA3	1:A:320:ASP:OD2	1.95	0.67
1:A:288:SER:N	1:A:289:PRO:CD	2.57	0.67
1:B:218:LEU:HD22	1:B:234:PHE:HD1	1.60	0.66
1:C:263:GLY:HA2	1:C:285:ASN:HB3	1.78	0.66
1:A:250:ARG:HH11	1:A:250:ARG:HB2	1.61	0.66
1:B:259:ILE:HD11	1:B:261:ILE:HD12	1.75	0.66
1:C:290:ASP:CG	1:C:290:ASP:O	2.37	0.66
1:A:334:VAL:HG12	1:A:335:VAL:N	2.09	0.66
1:B:81:SER:O	1:B:202:GLY:HA3	1.96	0.66
1:C:259:ILE:HG23	1:C:260:GLY:H	1.61	0.66
1:C:285:ASN:ND2	1:C:285:ASN:C	2.52	0.66
1:B:255:ILE:HD12	1:B:326:ARG:HH12	1.60	0.65
1:B:177:GLY:HA3	1:B:189:PHE:O	1.97	0.65
1:B:180:GLY:HA3	1:B:320:ASP:OD2	1.98	0.64
1:A:288:SER:O	1:A:289:PRO:C	2.40	0.64
1:B:260:GLY:O	1:B:289:PRO:CG	2.41	0.64
1:B:59:VAL:HG12	1:B:60:ASN:N	2.11	0.64
1:C:118:LEU:HD23	1:C:120:GLY:N	2.13	0.64
1:A:292:PRO:HD2	1:A:349:GLN:OE1	1.95	0.64
1:C:261:ILE:HG22	1:C:262:GLY:N	2.11	0.64
1:C:250:ARG:HB2	1:C:250:ARG:NH1	2.12	0.64
1:A:155:VAL:HG22	1:A:205:LEU:HD22	1.80	0.64
1:C:287:VAL:C	1:C:289:PRO:HD3	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:THR:O	1:C:218:LEU:CB	2.39	0.63
1:C:308:ASP:OD2	1:C:331:ILE:CG2	2.46	0.63
1:A:59:VAL:HG12	1:A:60:ASN:N	2.13	0.63
1:A:225:ASP:C	1:A:227:GLU:H	2.06	0.63
1:C:177:GLY:HA3	1:C:189:PHE:O	1.98	0.63
1:C:180:GLY:HA3	1:C:320:ASP:OD2	1.99	0.62
1:A:308:ASP:OD2	1:A:331:ILE:CG2	2.48	0.62
1:B:260:GLY:C	1:B:289:PRO:CG	2.70	0.62
1:B:78:THR:CG2	1:B:79:LEU:H	2.01	0.62
1:A:220:PHE:CD1	1:A:229:PRO:CB	2.83	0.62
1:A:222:LYS:CD	1:B:162:TYR:CD2	2.67	0.62
1:B:160:ASN:ND2	1:B:165:GLY:H	1.97	0.62
1:A:259:ILE:HB	1:A:322:VAL:HG11	1.81	0.61
1:C:94:ASN:OD1	1:C:201:SER:HB3	2.00	0.61
1:A:227:GLU:OE1	1:B:162:TYR:OH	2.17	0.61
1:B:250:ARG:HB2	1:B:250:ARG:HH11	1.65	0.61
1:A:65:GLY:HA3	1:A:77:ARG:HD3	1.82	0.61
1:A:160:ASN:ND2	1:A:165:GLY:H	1.98	0.61
1:A:220:PHE:HD1	1:A:229:PRO:HB2	1.65	0.61
1:A:239:GLN:HA	1:A:239:GLN:NE2	2.16	0.61
1:B:93:THR:HG23	1:B:128:ALA:HB3	1.83	0.61
1:B:94:ASN:HB2	1:B:97:VAL:HG23	1.82	0.61
1:B:178:ARG:HH11	1:B:178:ARG:CB	2.12	0.61
1:B:261:ILE:HG22	1:B:262:GLY:H	1.63	0.61
1:C:289:PRO:O	1:C:289:PRO:CD	2.49	0.61
1:A:96:HIS:ND1	1:A:126:ASP:OD2	2.29	0.61
1:A:122:ASP:CG	1:A:256:ARG:HH22	2.09	0.61
1:A:307:VAL:HG11	1:A:318:THR:HG23	1.83	0.61
1:C:59:VAL:HG12	1:C:60:ASN:N	2.15	0.61
1:B:55:ALA:HB1	1:B:166:GLN:HE22	1.66	0.61
1:A:42:MET:HE1	1:C:53:ARG:HH12	1.66	0.60
1:C:259:ILE:HG23	1:C:260:GLY:N	2.16	0.60
1:A:225:ASP:CG	1:A:226:GLY:N	2.58	0.60
1:A:81:SER:O	1:A:202:GLY:HA3	2.02	0.60
1:A:282:ILE:HD12	1:A:315:ALA:HA	1.83	0.60
1:C:96:HIS:ND1	1:C:126:ASP:OD2	2.32	0.60
1:C:306:SER:OG	1:C:334:VAL:HG23	2.02	0.60
1:A:307:VAL:CG1	1:A:318:THR:HG23	2.30	0.60
1:C:281:GLY:HA3	1:C:303:LEU:HD21	1.84	0.60
1:A:124:LEU:HD13	1:A:183:PRO:HG3	1.82	0.60
1:C:49:LEU:HD11	1:C:53:ARG:NE	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD23	1:B:120:GLY:N	2.14	0.59
1:C:178:ARG:HH11	1:C:178:ARG:CB	2.12	0.59
1:A:124:LEU:HD12	1:A:256:ARG:CZ	2.31	0.59
1:A:155:VAL:HG21	1:A:205:LEU:HD13	1.84	0.59
1:C:93:THR:HG23	1:C:128:ALA:HB3	1.84	0.59
1:B:120:GLY:HA3	1:B:248:LEU:HD22	1.84	0.59
1:B:259:ILE:HG23	1:B:260:GLY:N	2.18	0.59
1:C:55:ALA:HB1	1:C:166:GLN:NE2	2.17	0.59
1:C:221:ASP:HB3	1:C:229:PRO:HG3	1.83	0.59
1:A:125:THR:O	1:A:236:ILE:HD11	2.02	0.59
1:A:281:GLY:HA3	1:A:303:LEU:HD21	1.84	0.59
1:B:257:GLY:N	1:B:323:ALA:HA	2.18	0.59
1:C:58:VAL:HG21	1:C:158:ILE:HG22	1.83	0.59
1:A:94:ASN:HB2	1:A:97:VAL:HG23	1.83	0.59
1:B:65:GLY:HA3	1:B:77:ARG:HD3	1.85	0.59
1:B:259:ILE:HG23	1:B:260:GLY:H	1.68	0.58
1:C:96:HIS:HD1	1:C:126:ASP:CG	2.10	0.58
1:C:160:ASN:HD21	1:C:165:GLY:H	1.51	0.58
1:C:282:ILE:HD12	1:C:315:ALA:HA	1.85	0.58
1:A:94:ASN:OD1	1:A:201:SER:HB3	2.03	0.58
1:B:300:VAL:O	1:B:300:VAL:HG22	2.04	0.58
1:C:197:ASN:N	1:C:200:ASN:HD22	1.97	0.58
1:A:46:SER:HB2	1:C:153:ASP:HA	1.83	0.58
1:A:257:GLY:N	1:A:323:ALA:HA	2.18	0.58
1:B:181:LEU:HD22	1:B:247:LYS:HE3	1.86	0.58
1:A:85:MET:HG3	1:A:92:ILE:HG13	1.85	0.58
1:A:300:VAL:HG22	1:A:300:VAL:O	2.04	0.58
1:A:220:PHE:O	1:A:229:PRO:CG	2.47	0.58
1:A:253:ARG:HH12	1:A:255:ILE:HG12	1.69	0.58
1:B:63:ASN:HD22	1:B:64:ARG:N	2.01	0.58
1:C:257:GLY:N	1:C:323:ALA:HA	2.18	0.58
1:A:63:ASN:HD22	1:A:64:ARG:N	2.02	0.57
1:B:124:LEU:HD12	1:B:256:ARG:CZ	2.34	0.57
1:B:282:ILE:HD12	1:B:315:ALA:HA	1.85	0.57
1:B:305:ILE:HG12	1:B:335:VAL:CB	2.33	0.57
1:C:78:THR:HG22	1:C:79:LEU:N	2.13	0.57
1:B:63:ASN:C	1:B:63:ASN:ND2	2.55	0.57
1:B:77:ARG:HH22	1:B:100:ASP:HB2	1.69	0.57
1:B:218:LEU:HD23	1:B:233:GLY:CA	2.27	0.57
1:B:348:ILE:HD12	1:B:348:ILE:N	2.19	0.57
1:C:103:GLN:HG2	1:C:104:ILE:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:CG2	1:B:284:VAL:HG13	2.35	0.57
1:C:155:VAL:HG22	1:C:205:LEU:HD22	1.87	0.57
1:C:305:ILE:HB	1:C:334:VAL:CB	2.34	0.57
1:A:263:GLY:HA3	1:A:283:VAL:O	2.05	0.57
1:C:112:ARG:HB3	1:C:114:PHE:CE1	2.39	0.57
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.69	0.56
1:B:55:ALA:HB1	1:B:166:GLN:NE2	2.20	0.56
1:A:207:ASN:HD22	1:A:213:MET:HE2	1.70	0.56
1:A:260:GLY:O	1:A:289:PRO:HG2	2.04	0.56
1:B:122:ASP:CG	1:B:256:ARG:HH22	2.13	0.56
1:C:124:LEU:HB3	1:C:183:PRO:HB3	1.86	0.56
1:A:239:GLN:HE21	1:A:239:GLN:CA	2.19	0.56
1:A:290:ASP:O	1:A:294:ALA:HB3	2.04	0.56
1:C:305:ILE:HG12	1:C:335:VAL:CB	2.35	0.56
1:A:178:ARG:HH11	1:A:178:ARG:CB	2.17	0.56
1:C:94:ASN:HB2	1:C:97:VAL:HG23	1.87	0.56
1:C:300:VAL:HG22	1:C:300:VAL:O	2.06	0.56
1:B:197:ASN:N	1:B:200:ASN:HD22	1.97	0.56
1:A:118:LEU:HD23	1:A:120:GLY:N	2.17	0.56
1:B:191:GLN:HE22	1:C:167:THR:CG2	2.18	0.56
1:B:303:LEU:O	1:B:335:VAL:C	2.49	0.56
1:A:288:SER:C	1:A:289:PRO:O	2.42	0.55
1:A:348:ILE:N	1:A:348:ILE:HD12	2.21	0.55
1:B:308:ASP:OD2	1:B:331:ILE:HB	2.06	0.55
1:C:295:ASN:O	1:C:296:ALA:CB	2.50	0.55
1:A:92:ILE:HG22	1:A:93:THR:N	2.20	0.55
1:B:85:MET:HG3	1:B:92:ILE:HG13	1.88	0.55
1:C:79:LEU:O	1:C:79:LEU:HD12	2.07	0.55
1:A:263:GLY:HA2	1:A:285:ASN:H	1.72	0.55
1:B:124:LEU:HB3	1:B:183:PRO:HB3	1.88	0.55
1:A:95:LYS:C	1:A:97:VAL:H	2.14	0.55
1:A:282:ILE:CD1	1:A:315:ALA:HA	2.35	0.55
1:A:290:ASP:O	1:A:291:GLY:C	2.49	0.55
1:B:282:ILE:CD1	1:B:315:ALA:HA	2.36	0.55
1:B:351:TYR:CG	1:B:352:PRO:HD2	2.41	0.55
1:B:288:SER:N	1:B:289:PRO:HD3	2.22	0.55
1:C:176:THR:O	1:C:190:LEU:HD12	2.07	0.55
1:A:129:VAL:HG23	1:A:248:LEU:HD12	1.89	0.55
1:B:53:ARG:HH22	1:C:42:MET:HE1	1.72	0.55
1:B:288:SER:N	1:B:289:PRO:CD	2.70	0.55
1:A:124:LEU:HB3	1:A:183:PRO:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HB	1:A:334:VAL:HB	1.90	0.54
1:C:288:SER:N	1:C:289:PRO:HD3	2.22	0.54
1:C:290:ASP:O	1:C:290:ASP:OD1	2.25	0.54
1:A:259:ILE:O	1:A:259:ILE:HG22	2.04	0.54
1:A:96:HIS:HD1	1:A:126:ASP:CG	2.14	0.54
1:A:222:LYS:HD3	1:B:162:TYR:CD2	2.42	0.54
1:A:78:THR:HG22	1:A:79:LEU:N	2.13	0.54
1:A:181:LEU:CD2	1:A:247:LYS:HE3	2.36	0.54
1:C:351:TYR:CG	1:C:352:PRO:HD2	2.42	0.54
1:B:239:GLN:NE2	1:B:239:GLN:HA	2.23	0.54
1:B:155:VAL:HG21	1:B:205:LEU:HD13	1.90	0.54
1:C:48:ASN:OD1	1:C:52:ARG:NH1	2.40	0.54
1:C:259:ILE:O	1:C:292:PRO:HG2	2.08	0.54
1:C:282:ILE:CD1	1:C:315:ALA:HA	2.37	0.54
1:C:288:SER:O	1:C:289:PRO:C	2.46	0.54
1:C:124:LEU:HD12	1:C:256:ARG:NH1	2.23	0.54
1:A:63:ASN:CG	1:A:101:ALA:HB2	2.33	0.54
1:B:58:VAL:HG21	1:B:158:ILE:HG22	1.90	0.54
1:B:308:ASP:OD2	1:B:331:ILE:CB	2.55	0.54
1:C:63:ASN:HD22	1:C:64:ARG:N	2.05	0.54
1:C:306:SER:OG	1:C:334:VAL:CG2	2.56	0.54
1:B:259:ILE:HB	1:B:322:VAL:HG11	1.89	0.53
1:C:253:ARG:HH12	1:C:255:ILE:HG12	1.70	0.53
1:A:103:GLN:HG2	1:A:104:ILE:N	2.23	0.53
1:A:255:ILE:CD1	1:A:326:ARG:HH12	2.20	0.53
1:C:259:ILE:HB	1:C:322:VAL:HG11	1.90	0.53
1:A:55:ALA:HB1	1:A:166:GLN:HE22	1.74	0.53
1:A:182:ASN:ND2	1:A:183:PRO:HD2	2.13	0.53
1:B:103:GLN:HG2	1:B:104:ILE:N	2.24	0.53
1:A:172:ILE:CG2	1:B:170:GLN:HG2	2.38	0.53
1:C:63:ASN:C	1:C:63:ASN:ND2	2.57	0.53
1:A:147:ARG:NH1	1:A:211:GLU:OE1	2.42	0.53
1:B:305:ILE:HB	1:B:334:VAL:CB	2.38	0.53
1:C:348:ILE:N	1:C:348:ILE:HD12	2.23	0.53
1:A:94:ASN:HB2	1:A:97:VAL:CG2	2.37	0.53
1:C:125:THR:O	1:C:236:ILE:HD11	2.08	0.53
1:A:305:ILE:HB	1:A:334:VAL:CB	2.39	0.52
1:A:291:GLY:O	1:A:295:ASN:ND2	2.41	0.52
1:A:65:GLY:H	1:A:77:ARG:HG3	1.74	0.52
1:C:65:GLY:HA3	1:C:77:ARG:HD3	1.91	0.52
1:C:181:LEU:HD22	1:C:247:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:OD1	1:C:202:GLY:N	2.42	0.52
1:C:255:ILE:CD1	1:C:326:ARG:HH12	2.23	0.52
1:B:263:GLY:HA3	1:B:283:VAL:O	2.09	0.52
1:B:306:SER:OG	1:B:334:VAL:HG23	2.09	0.52
1:C:284:VAL:HB	1:C:302:ASP:O	2.09	0.52
1:A:304:ILE:HA	1:A:335:VAL:C	2.35	0.52
1:B:207:ASN:ND2	1:B:213:MET:HE2	2.24	0.52
1:C:218:LEU:C	1:C:218:LEU:CD1	2.51	0.52
1:A:351:TYR:CG	1:A:352:PRO:HD2	2.45	0.52
1:B:47:TYR:CE2	1:B:154:VAL:HG11	2.45	0.52
1:C:83:VAL:CG2	1:C:204:ALA:HB2	2.40	0.52
1:A:153:ASP:HA	1:B:46:SER:HB2	1.90	0.51
1:A:284:VAL:HB	1:A:302:ASP:O	2.10	0.51
1:C:206:VAL:HG12	1:C:212:LEU:HA	1.91	0.51
1:A:58:VAL:HG21	1:A:158:ILE:HG22	1.91	0.51
1:C:65:GLY:H	1:C:77:ARG:HG3	1.75	0.51
1:C:284:VAL:HG12	1:C:284:VAL:O	2.10	0.51
1:C:305:ILE:HB	1:C:334:VAL:CG1	2.39	0.51
1:B:261:ILE:CG2	1:B:262:GLY:N	2.74	0.51
1:C:261:ILE:HG22	1:C:262:GLY:H	1.73	0.51
1:C:92:ILE:HG22	1:C:93:THR:N	2.25	0.51
1:B:59:VAL:CG1	1:B:60:ASN:N	2.73	0.51
1:C:47:TYR:HB3	1:C:156:LEU:HD11	1.92	0.51
1:C:288:SER:N	1:C:289:PRO:CD	2.73	0.51
1:A:47:TYR:HB3	1:A:156:LEU:HD11	1.91	0.51
1:B:304:ILE:HA	1:B:335:VAL:C	2.35	0.51
1:A:86:ASP:OD2	1:A:86:ASP:C	2.54	0.51
1:A:161:PRO:HB2	1:A:197:ASN:HB2	1.92	0.51
1:A:55:ALA:HB1	1:A:166:GLN:NE2	2.25	0.51
1:A:104:ILE:HG21	1:A:130:LEU:HD13	1.92	0.51
1:A:63:ASN:C	1:A:63:ASN:ND2	2.54	0.51
1:A:95:LYS:O	1:A:97:VAL:N	2.44	0.51
1:B:96:HIS:ND1	1:B:126:ASP:OD2	2.39	0.51
1:A:260:GLY:O	1:A:293:ALA:HB2	2.11	0.51
1:B:162:TYR:HE1	1:B:197:ASN:HB3	1.75	0.50
1:B:181:LEU:CD2	1:B:247:LYS:HE3	2.40	0.50
1:A:250:ARG:HB2	1:A:250:ARG:NH1	2.25	0.50
1:C:224:ASN:CG	1:C:225:ASP:N	2.70	0.50
1:A:263:GLY:HA2	1:A:285:ASN:HB3	1.94	0.50
1:B:59:VAL:CG1	1:B:106:VAL:HG13	2.18	0.50
1:B:250:ARG:HB2	1:B:250:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:HH22	1:C:100:ASP:HB2	1.77	0.50
1:A:161:PRO:CB	1:A:197:ASN:HB2	2.40	0.50
1:A:42:MET:HE3	1:C:209:LEU:HD22	1.92	0.50
1:B:48:ASN:OD1	1:B:52:ARG:NH1	2.45	0.50
1:B:230:GLU:HG2	1:B:231:GLY:N	2.27	0.50
1:C:83:VAL:HG21	1:C:204:ALA:HB2	1.92	0.50
1:A:330:VAL:CG2	1:A:347:THR:HG22	2.34	0.50
1:B:92:ILE:HG22	1:B:93:THR:N	2.27	0.50
1:B:281:GLY:HA3	1:B:303:LEU:HD21	1.92	0.50
1:A:220:PHE:CD1	1:A:229:PRO:HG3	2.47	0.49
1:A:304:ILE:HD13	1:A:335:VAL:C	2.37	0.49
1:B:125:THR:O	1:B:236:ILE:HD11	2.11	0.49
1:C:122:ASP:CG	1:C:256:ARG:HH22	2.21	0.49
1:A:85:MET:CG	1:A:92:ILE:HG13	2.42	0.49
1:B:186:ARG:HA	1:B:189:PHE:CE2	2.47	0.49
1:B:261:ILE:CG2	1:B:262:GLY:H	2.25	0.49
1:C:55:ALA:HB1	1:C:166:GLN:HE22	1.77	0.49
1:B:147:ARG:NH1	1:B:211:GLU:OE1	2.44	0.49
1:C:263:GLY:HA3	1:C:283:VAL:O	2.12	0.49
1:A:120:GLY:HA3	1:A:248:LEU:HD22	1.94	0.49
1:A:191:GLN:HE22	1:B:167:THR:CG2	2.25	0.49
1:B:284:VAL:HB	1:B:302:ASP:O	2.12	0.49
1:C:92:ILE:CG2	1:C:93:THR:N	2.75	0.49
1:C:307:VAL:CG1	1:C:318:THR:HG23	2.41	0.49
1:C:307:VAL:O	1:C:308:ASP:C	2.53	0.49
1:A:334:VAL:CG1	1:A:335:VAL:H	2.18	0.49
1:A:79:LEU:O	1:A:79:LEU:HD12	2.13	0.49
1:B:63:ASN:CG	1:B:101:ALA:HB2	2.38	0.49
1:B:287:VAL:C	1:B:289:PRO:HD3	2.37	0.49
1:C:119:VAL:HG23	1:C:119:VAL:O	2.13	0.49
1:A:224:ASN:CG	1:A:225:ASP:N	2.69	0.49
1:B:92:ILE:CG2	1:B:93:THR:N	2.76	0.49
1:B:284:VAL:CG2	1:B:304:ILE:HG12	2.43	0.49
1:C:94:ASN:HB2	1:C:97:VAL:CG2	2.43	0.49
1:B:104:ILE:HG21	1:B:130:LEU:HD13	1.94	0.49
1:B:295:ASN:O	1:B:296:ALA:CB	2.53	0.49
1:C:222:LYS:C	1:C:224:ASN:H	2.20	0.49
1:A:207:ASN:HB3	1:A:213:MET:HE2	1.95	0.49
1:B:96:HIS:HD1	1:B:126:ASP:CG	2.21	0.49
1:B:174:SER:HB3	1:C:168:ILE:H	1.77	0.48
1:C:63:ASN:HD21	1:C:101:ALA:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:CG2	1:B:347:THR:HG22	2.38	0.48
1:C:261:ILE:CG2	1:C:262:GLY:N	2.77	0.48
1:C:304:ILE:HA	1:C:335:VAL:C	2.38	0.48
1:C:151:ILE:CD1	1:C:175:ALA:HA	2.44	0.48
1:A:92:ILE:CG2	1:A:93:THR:N	2.75	0.48
1:B:253:ARG:HH12	1:B:255:ILE:HG12	1.76	0.48
1:C:104:ILE:HG21	1:C:130:LEU:HD13	1.94	0.48
1:C:239:GLN:NE2	1:C:239:GLN:HA	2.28	0.48
1:A:206:VAL:HG12	1:A:212:LEU:HA	1.96	0.48
1:C:207:ASN:HB3	1:C:213:MET:HE2	1.96	0.48
1:A:292:PRO:O	1:A:293:ALA:C	2.55	0.48
1:B:263:GLY:HA2	1:B:285:ASN:CB	2.44	0.48
1:C:261:ILE:CG2	1:C:284:VAL:HG13	2.43	0.48
1:A:55:ALA:N	1:A:56:PRO:CD	2.76	0.48
1:C:147:ARG:NH1	1:C:211:GLU:OE1	2.47	0.48
1:C:308:ASP:OD2	1:C:331:ILE:HB	2.13	0.48
1:B:182:ASN:ND2	1:B:183:PRO:HD2	2.18	0.48
1:C:95:LYS:C	1:C:97:VAL:H	2.22	0.47
1:A:46:SER:CB	1:C:153:ASP:HA	2.44	0.47
1:A:47:TYR:CE2	1:A:154:VAL:HG11	2.49	0.47
1:A:220:PHE:CE1	1:A:222:LYS:HD3	2.49	0.47
1:B:263:GLY:HA2	1:B:285:ASN:HB2	1.96	0.47
1:C:112:ARG:HB3	1:C:114:PHE:HE1	1.79	0.47
1:A:53:ARG:HH22	1:B:42:MET:HE1	1.79	0.47
1:B:257:GLY:HA3	1:B:322:VAL:O	2.14	0.47
1:B:260:GLY:CA	1:B:289:PRO:HG2	2.43	0.47
1:C:85:MET:HG3	1:C:92:ILE:HG13	1.94	0.47
1:C:257:GLY:H	1:C:323:ALA:CA	2.27	0.47
1:C:303:LEU:O	1:C:335:VAL:C	2.58	0.47
1:A:305:ILE:HB	1:A:334:VAL:HG11	1.97	0.47
1:B:104:ILE:HG21	1:B:130:LEU:CD1	2.45	0.47
1:B:209:LEU:HD22	1:C:42:MET:HE3	1.96	0.47
1:C:141:ILE:HG23	1:C:141:ILE:O	2.13	0.47
1:A:112:ARG:HB3	1:A:114:PHE:CE1	2.50	0.47
1:A:300:VAL:O	1:A:301:ASN:HB2	2.15	0.47
1:C:59:VAL:CG1	1:C:60:ASN:N	2.78	0.47
1:C:284:VAL:CG2	1:C:304:ILE:HG12	2.44	0.47
1:A:120:GLY:O	1:A:248:LEU:HD13	2.15	0.47
1:B:94:ASN:HB2	1:B:97:VAL:CG2	2.45	0.47
1:C:297:GLY:O	1:C:298:ILE:O	2.33	0.47
1:B:59:VAL:HG11	1:B:106:VAL:CG1	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:N	1:B:126:ASP:O	2.45	0.47
1:C:113:VAL:C	1:C:114:PHE:CD1	2.93	0.47
1:A:93:THR:HG23	1:A:128:ALA:HB3	1.97	0.47
1:B:160:ASN:C	1:B:160:ASN:HD22	2.22	0.47
1:A:121:SER:O	1:A:248:LEU:HD21	2.15	0.46
1:C:117:LEU:HD13	1:C:119:VAL:HG12	1.96	0.46
1:C:250:ARG:NH1	1:C:250:ARG:CB	2.75	0.46
1:A:58:VAL:HG22	1:A:166:GLN:OE1	2.15	0.46
1:B:218:LEU:HD13	1:B:219:SER:H	1.64	0.46
1:B:239:GLN:HE21	1:B:239:GLN:CA	2.27	0.46
1:A:59:VAL:CG1	1:A:60:ASN:N	2.77	0.46
1:A:220:PHE:CD1	1:A:229:PRO:CG	2.98	0.46
1:B:121:SER:O	1:B:248:LEU:HD21	2.15	0.46
1:B:239:GLN:HA	1:B:239:GLN:HE21	1.79	0.46
1:C:181:LEU:CD2	1:C:247:LYS:HE3	2.45	0.46
1:B:94:ASN:OD1	1:B:201:SER:HB3	2.15	0.46
1:B:129:VAL:HG23	1:B:248:LEU:CD1	2.42	0.46
1:B:230:GLU:O	1:B:232:ILE:HG13	2.16	0.46
1:C:49:LEU:HD11	1:C:53:ARG:HE	1.80	0.46
1:C:93:THR:O	1:C:128:ALA:N	2.41	0.46
1:B:147:ARG:HH11	1:B:211:GLU:CD	2.23	0.46
1:C:79:LEU:HD12	1:C:79:LEU:C	2.41	0.46
1:B:55:ALA:N	1:B:56:PRO:CD	2.79	0.46
1:C:287:VAL:C	1:C:289:PRO:CD	2.88	0.46
1:A:261:ILE:HG23	1:A:284:VAL:HG13	1.98	0.46
1:B:161:PRO:HA	1:B:199:GLY:CA	2.41	0.46
1:C:55:ALA:N	1:C:56:PRO:CD	2.78	0.46
1:C:86:ASP:OD2	1:C:86:ASP:C	2.59	0.46
1:B:307:VAL:CG1	1:B:318:THR:HG23	2.45	0.46
1:A:110:ASP:OD1	1:A:110:ASP:C	2.57	0.46
1:A:220:PHE:HD1	1:A:229:PRO:CG	2.29	0.46
1:B:93:THR:O	1:B:128:ALA:N	2.45	0.46
1:B:95:LYS:C	1:B:97:VAL:H	2.23	0.46
1:B:287:VAL:C	1:B:289:PRO:CD	2.89	0.46
1:C:218:LEU:C	1:C:218:LEU:HD22	2.41	0.46
1:B:206:VAL:HG12	1:B:212:LEU:HA	1.98	0.45
1:A:261:ILE:HG22	1:A:262:GLY:N	2.31	0.45
1:B:284:VAL:O	1:B:284:VAL:HG12	2.15	0.45
1:A:79:LEU:HD12	1:A:79:LEU:C	2.41	0.45
1:B:158:ILE:HG23	1:B:168:ILE:CD1	2.47	0.45
1:B:218:LEU:HD22	1:B:234:PHE:CD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD12	1:C:256:ARG:CZ	2.45	0.45
1:A:95:LYS:C	1:A:97:VAL:N	2.72	0.45
1:A:117:LEU:HD13	1:A:119:VAL:HG12	1.98	0.45
1:A:184:THR:CB	1:A:188:ASN:HD22	2.29	0.45
1:A:287:VAL:C	1:A:289:PRO:HD3	2.41	0.45
1:B:65:GLY:H	1:B:77:ARG:HG3	1.81	0.45
1:B:305:ILE:HB	1:B:334:VAL:CG1	2.46	0.45
1:C:257:GLY:HA3	1:C:322:VAL:O	2.17	0.45
1:C:300:VAL:O	1:C:301:ASN:HB2	2.16	0.45
1:A:258:TYR:CZ	1:A:260:GLY:HA3	2.52	0.45
1:B:257:GLY:O	1:B:322:VAL:HG12	2.16	0.45
1:C:103:GLN:HG2	1:C:104:ILE:H	1.82	0.45
1:A:158:ILE:HG12	1:A:168:ILE:HD12	1.97	0.45
1:B:134:ALA:HB3	1:B:138:LEU:HG	1.98	0.45
1:B:65:GLY:N	1:B:77:ARG:HG3	2.31	0.45
1:B:263:GLY:HA2	1:B:285:ASN:H	1.82	0.44
1:B:218:LEU:HD13	1:B:219:SER:C	2.42	0.44
1:C:93:THR:CG2	1:C:128:ALA:HB3	2.46	0.44
1:C:122:ASP:OD2	1:C:125:THR:HG23	2.17	0.44
1:B:127:LEU:HG	1:B:236:ILE:HD13	1.99	0.44
1:C:95:LYS:O	1:C:97:VAL:N	2.50	0.44
1:A:117:LEU:HD22	1:A:118:LEU:N	2.33	0.44
1:B:151:ILE:CD1	1:B:175:ALA:HA	2.47	0.44
1:B:160:ASN:ND2	1:B:160:ASN:C	2.75	0.44
1:B:308:ASP:OD2	1:B:331:ILE:HG22	2.14	0.44
1:A:224:ASN:CG	1:A:225:ASP:H	2.26	0.44
1:B:141:ILE:O	1:B:141:ILE:HG23	2.16	0.44
1:C:47:TYR:CE2	1:C:154:VAL:HG11	2.53	0.44
1:C:218:LEU:HD22	1:C:219:SER:N	2.32	0.44
1:B:122:ASP:OD2	1:B:125:THR:HG23	2.17	0.44
1:A:305:ILE:HB	1:A:334:VAL:CG1	2.48	0.44
1:C:78:THR:O	1:C:79:LEU:HB3	2.18	0.44
1:C:123:SER:C	1:C:125:THR:H	2.25	0.44
1:C:158:ILE:HG12	1:C:168:ILE:HD12	2.00	0.43
1:A:170:GLN:O	1:A:170:GLN:HG3	2.17	0.43
1:B:165:GLY:O	1:B:167:THR:HG23	2.17	0.43
1:B:236:ILE:O	1:B:237:PRO:C	2.61	0.43
1:C:182:ASN:ND2	1:C:183:PRO:HD2	2.18	0.43
1:B:86:ASP:C	1:B:86:ASP:OD2	2.60	0.43
1:B:218:LEU:CD2	1:B:234:PHE:HD1	2.30	0.43
1:C:147:ARG:HH11	1:C:211:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HH11	1:A:211:GLU:CD	2.26	0.43
1:A:153:ASP:HA	1:B:46:SER:CB	2.48	0.43
1:B:300:VAL:O	1:B:301:ASN:HB2	2.18	0.43
1:C:308:ASP:OD2	1:C:331:ILE:HG22	2.18	0.43
1:A:148:VAL:HA	1:A:149:PRO:HD3	1.85	0.43
1:B:78:THR:O	1:B:79:LEU:HB3	2.18	0.43
1:A:219:SER:OG	1:A:220:PHE:N	2.52	0.43
1:B:176:THR:O	1:B:190:LEU:HD12	2.18	0.43
1:A:63:ASN:ND2	1:A:101:ALA:CB	2.82	0.43
1:A:151:ILE:CD1	1:A:175:ALA:HA	2.49	0.43
1:B:170:GLN:HE22	1:C:170:GLN:HE22	1.67	0.43
1:B:218:LEU:CD2	1:B:233:GLY:HA2	2.31	0.43
1:C:308:ASP:H	1:C:331:ILE:HD12	1.84	0.43
1:A:250:ARG:NH1	1:A:250:ARG:CB	2.82	0.43
1:C:68:THR:OG1	1:C:77:ARG:HG2	2.18	0.43
1:C:141:ILE:O	1:C:141:ILE:CG2	2.64	0.43
1:A:160:ASN:C	1:A:160:ASN:HD22	2.26	0.42
1:A:331:ILE:O	1:A:331:ILE:HG13	2.17	0.42
1:A:58:VAL:HG11	1:A:158:ILE:HB	2.01	0.42
1:A:303:LEU:C	1:A:303:LEU:HD23	2.43	0.42
1:A:331:ILE:HG12	1:A:348:ILE:HD11	2.00	0.42
1:B:351:TYR:CD2	1:B:352:PRO:HD2	2.54	0.42
1:C:59:VAL:HG13	1:C:107:ALA:C	2.43	0.42
1:C:261:ILE:CG2	1:C:262:GLY:H	2.31	0.42
1:B:98:ILE:HG21	1:B:104:ILE:HD13	2.02	0.42
1:C:186:ARG:HA	1:C:189:PHE:CE2	2.55	0.42
1:A:207:ASN:ND2	1:A:213:MET:HE2	2.33	0.42
1:C:162:TYR:HE1	1:C:197:ASN:HB3	1.84	0.42
1:A:141:ILE:O	1:A:141:ILE:HG23	2.19	0.42
1:A:167:THR:HG21	1:C:191:GLN:HE22	1.84	0.42
1:A:63:ASN:HD21	1:A:101:ALA:HA	1.83	0.42
1:A:176:THR:O	1:A:190:LEU:HD12	2.19	0.42
1:A:306:SER:OG	1:A:334:VAL:HG23	2.20	0.42
1:C:291:GLY:O	1:C:295:ASN:ND2	2.52	0.42
1:C:65:GLY:N	1:C:77:ARG:HG3	2.34	0.42
1:C:260:GLY:C	1:C:289:PRO:CG	2.87	0.42
1:B:144:ASN:OD1	1:B:144:ASN:C	2.62	0.42
1:B:161:PRO:C	1:B:163:ASN:N	2.77	0.42
1:C:63:ASN:CG	1:C:101:ALA:HB2	2.44	0.42
1:A:308:ASP:OD2	1:A:331:ILE:HG21	2.19	0.42
1:B:47:TYR:HB3	1:B:156:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ALA:CB	1:B:138:LEU:HG	2.50	0.42
1:C:58:VAL:HG11	1:C:158:ILE:HB	2.02	0.42
1:C:263:GLY:HA2	1:C:285:ASN:H	1.85	0.42
1:A:42:MET:CE	1:C:209:LEU:HD22	2.50	0.41
1:A:182:ASN:HD22	1:A:183:PRO:N	2.17	0.41
1:C:184:THR:OG1	1:C:188:ASN:HB2	2.20	0.41
1:C:303:LEU:C	1:C:303:LEU:HD23	2.45	0.41
1:C:54:ALA:HB1	1:C:141:ILE:HD11	2.02	0.41
1:A:148:VAL:HG13	1:A:150:HIS:CE1	2.56	0.41
1:C:158:ILE:HG23	1:C:168:ILE:CD1	2.50	0.41
1:C:307:VAL:CG2	1:C:318:THR:HG23	2.50	0.41
1:A:259:ILE:CD1	1:A:261:ILE:HD12	2.38	0.41
1:B:257:GLY:H	1:B:323:ALA:CA	2.28	0.41
1:C:94:ASN:O	1:C:97:VAL:HG23	2.19	0.41
1:C:239:GLN:HE21	1:C:239:GLN:CA	2.34	0.41
1:A:65:GLY:N	1:A:77:ARG:HG3	2.34	0.41
1:A:77:ARG:HH22	1:A:100:ASP:HB2	1.84	0.41
1:A:284:VAL:CG2	1:A:304:ILE:HG12	2.51	0.41
1:B:90:TYR:CE2	1:B:131:LYS:HD2	2.54	0.41
1:B:172:ILE:HG23	1:C:170:GLN:HG2	2.03	0.41
1:C:207:ASN:HD22	1:C:213:MET:HE2	1.86	0.41
1:C:251:ASP:CG	1:C:326:ARG:HH22	2.29	0.41
1:C:331:ILE:HG12	1:C:348:ILE:HD11	2.03	0.41
1:A:64:ARG:HA	1:A:75:GLU:O	2.21	0.41
1:C:248:LEU:HD23	1:C:248:LEU:HA	1.87	0.41
1:A:184:THR:OG1	1:A:188:ASN:HB2	2.21	0.41
1:A:284:VAL:HG12	1:A:284:VAL:O	2.19	0.41
1:A:287:VAL:C	1:A:289:PRO:CD	2.94	0.41
1:B:155:VAL:CG2	1:B:205:LEU:HD22	2.48	0.41
1:B:186:ARG:HA	1:B:189:PHE:CD2	2.56	0.41
1:B:261:ILE:HG23	1:B:284:VAL:HG13	2.02	0.41
1:C:85:MET:HG3	1:C:245:MET:SD	2.60	0.41
1:B:58:VAL:HG11	1:B:158:ILE:HB	2.03	0.41
1:B:95:LYS:C	1:B:97:VAL:N	2.79	0.41
1:B:122:ASP:OD2	1:B:256:ARG:NH2	2.48	0.41
1:B:175:ALA:HB3	1:B:191:GLN:HB3	2.03	0.41
1:B:184:THR:OG1	1:B:188:ASN:HB2	2.21	0.40
1:B:218:LEU:C	1:B:218:LEU:HD12	2.38	0.40
1:C:125:THR:O	1:C:236:ILE:CD1	2.68	0.40
1:B:158:ILE:HG23	1:B:168:ILE:HD13	2.03	0.40
1:A:161:PRO:HA	1:A:199:GLY:CA	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLY:H	1:A:323:ALA:CA	2.28	0.40
1:C:310:LYS:HG3	1:C:311:PRO:CD	2.45	0.40
1:A:220:PHE:HE1	1:A:222:LYS:HD3	1.87	0.40
1:B:94:ASN:CA	1:B:126:ASP:O	2.67	0.40
1:B:119:VAL:O	1:B:119:VAL:HG23	2.20	0.40
1:C:55:ALA:HB3	1:C:56:PRO:HD3	2.03	0.40
1:B:119:VAL:HG22	1:B:129:VAL:HB	2.04	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:C	1:B:53:ARG:NH2[1_556]	1.48	0.72
1:A:225:ASP:N	1:B:53:ARG:NH2[1_556]	1.75	0.45
1:A:224:ASN:O	1:B:53:ARG:NH2[1_556]	1.86	0.34
1:A:225:ASP:OD1	1:C:42:MET:CE[1_556]	1.94	0.26
1:A:225:ASP:CB	1:B:53:ARG:NH1[1_556]	2.03	0.17

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	285/314 (91%)	234 (82%)	39 (14%)	12 (4%)	2	10
1	B	285/314 (91%)	233 (82%)	37 (13%)	15 (5%)	1	7
1	C	285/314 (91%)	235 (82%)	39 (14%)	11 (4%)	2	11
All	All	855/942 (91%)	702 (82%)	115 (14%)	38 (4%)	2	9

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLY

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	296	ALA
1	A	298	ILE
1	A	334	VAL
1	B	220	PHE
1	B	227	GLU
1	B	285	ASN
1	B	298	ILE
1	C	295	ASN
1	C	296	ALA
1	C	298	ILE
1	A	222	LYS
1	A	301	ASN
1	B	223	SER
1	B	291	GLY
1	B	296	ALA
1	B	301	ASN
1	C	96	HIS
1	C	301	ASN
1	A	96	HIS
1	A	124	LEU
1	C	124	LEU
1	C	222	LYS
1	B	96	HIS
1	B	124	LEU
1	B	162	TYR
1	C	218	LEU
1	A	351	TYR
1	B	343	THR
1	B	351	TYR
1	C	343	THR
1	A	72	ASN
1	A	343	THR
1	B	295	ASN
1	C	308	ASP
1	B	288	SER
1	C	351	TYR

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	225/253 (89%)	205 (91%)	20 (9%)	9	29
1	B	225/253 (89%)	209 (93%)	16 (7%)	13	37
1	C	225/253 (89%)	208 (92%)	17 (8%)	12	35
All	All	675/759 (89%)	622 (92%)	53 (8%)	11	34

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	63	ASN
1	A	70	SER
1	A	87	GLN
1	A	117	LEU
1	A	119	VAL
1	A	135	THR
1	A	170	GLN
1	A	190	LEU
1	A	205	LEU
1	A	218	LEU
1	A	222	LYS
1	A	227	GLU
1	A	240	LEU
1	A	259	ILE
1	A	285	ASN
1	A	286	GLU
1	A	290	ASP
1	A	302	ASP
1	A	307	VAL
1	B	63	ASN
1	B	117	LEU
1	B	119	VAL
1	B	135	THR
1	B	190	LEU
1	B	205	LEU
1	B	218	LEU
1	B	219	SER
1	B	224	ASN
1	B	227	GLU

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Mol	Chain	Res	Type
1	B	240	LEU
1	B	286	GLU
1	B	290	ASP
1	B	302	ASP
1	B	307	VAL
1	B	308	ASP
1	C	63	ASN
1	C	87	GLN
1	C	117	LEU
1	C	119	VAL
1	C	135	THR
1	C	148	VAL
1	C	205	LEU
1	C	218	LEU
1	C	224	ASN
1	C	227	GLU
1	C	240	LEU
1	C	242	THR
1	C	285	ASN
1	C	286	GLU
1	C	290	ASP
1	C	302	ASP
1	C	307	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	63	ASN
1	A	73	GLN
1	A	160	ASN
1	A	163	ASN
1	A	166	GLN
1	A	170	GLN
1	A	182	ASN
1	A	188	ASN
1	A	191	GLN
1	A	197	ASN
1	A	200	ASN
1	A	216	ASN
1	A	224	ASN
1	A	239	GLN

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	299	GLN
1	A	309	ASN
1	A	321	GLN
1	A	345	GLN
1	B	60	ASN
1	B	63	ASN
1	B	72	ASN
1	B	73	GLN
1	B	109	GLN
1	B	160	ASN
1	B	163	ASN
1	B	182	ASN
1	B	188	ASN
1	B	191	GLN
1	B	200	ASN
1	B	216	ASN
1	B	239	GLN
1	B	295	ASN
1	B	309	ASN
1	B	345	GLN
1	C	60	ASN
1	C	63	ASN
1	C	73	GLN
1	C	160	ASN
1	C	163	ASN
1	C	170	GLN
1	C	182	ASN
1	C	188	ASN
1	C	191	GLN
1	C	197	ASN
1	C	200	ASN
1	C	216	ASN
1	C	239	GLN
1	C	295	ASN
1	C	299	GLN
1	C	309	ASN
1	C	345	GLN

5.3.3 RNA ⓘ

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	224:ASN	C	225:ASP	N	0.88

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	291/314 (92%)	-0.02	13 (4%)	38 20	17, 55, 156, 176	0
1	B	285/314 (90%)	0.15	14 (4%)	35 17	22, 71, 167, 179	1 (0%)
1	C	291/314 (92%)	0.35	25 (8%)	16 9	27, 81, 179, 191	0
All	All	867/942 (92%)	0.16	52 (5%)	27 14	17, 70, 172, 191	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ASP	5.6
1	B	261	ILE	5.5
1	A	221	ASP	4.8
1	B	227	GLU	4.5
1	A	220	PHE	3.8
1	A	227	GLU	3.7
1	B	219	SER	3.6
1	C	346	VAL	3.5
1	C	68	THR	3.5
1	C	259	ILE	3.2
1	B	133	ASN	3.1
1	C	307	VAL	3.1
1	A	226	GLY	3.1
1	B	226	GLY	3.0
1	B	264	ARG	3.0
1	B	259	ILE	2.9
1	C	304	ILE	2.9
1	A	264	ARG	2.8
1	C	313	ILE	2.8
1	C	67	ASN	2.8
1	A	223	SER	2.7
1	C	66	LEU	2.7
1	A	219	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	222	LYS	2.6
1	C	305	ILE	2.6
1	C	316	LEU	2.6
1	A	224	ASN	2.6
1	C	261	ILE	2.5
1	A	261	ILE	2.4
1	C	314	SER	2.4
1	A	334	VAL	2.3
1	C	348	ILE	2.3
1	C	347	THR	2.2
1	C	298	ILE	2.2
1	B	300	VAL	2.2
1	C	181	LEU	2.2
1	B	333	VAL	2.2
1	C	78	THR	2.2
1	B	293	ALA	2.2
1	A	262	GLY	2.2
1	C	250	ARG	2.2
1	B	254	VAL	2.1
1	C	331	ILE	2.1
1	B	305	ILE	2.1
1	B	135	THR	2.1
1	C	303	LEU	2.1
1	C	343	THR	2.1
1	B	136	GLY	2.1
1	C	65	GLY	2.1
1	C	300	VAL	2.0
1	C	330	VAL	2.0
1	C	311	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.