



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:14 AM UTC

PDB ID : 5CH6 / pdb_00005ch6
Title : Crystal Structure of FRIGIDA Flowering-time Regulator
Authors : Hyun, K.; Song, J.J.
Deposited on : 2015-07-10
Resolution : 3.26 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

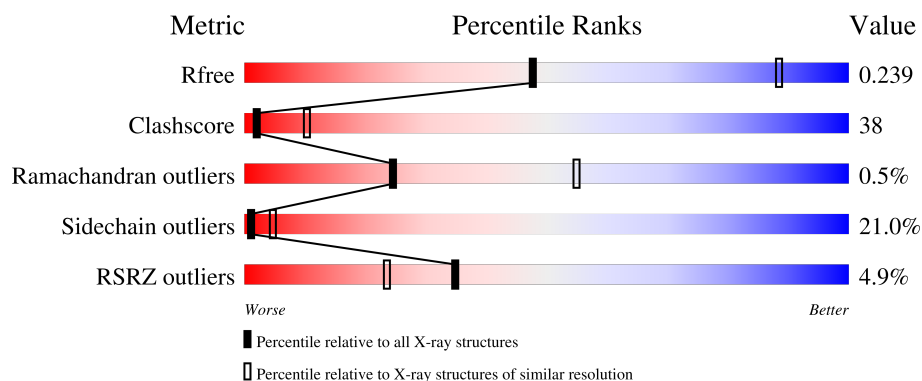
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	289	4% 41% 45% 12%
1	B	289	7% 42% 42% 15%
1	C	289	4% 38% 45% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6819 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.

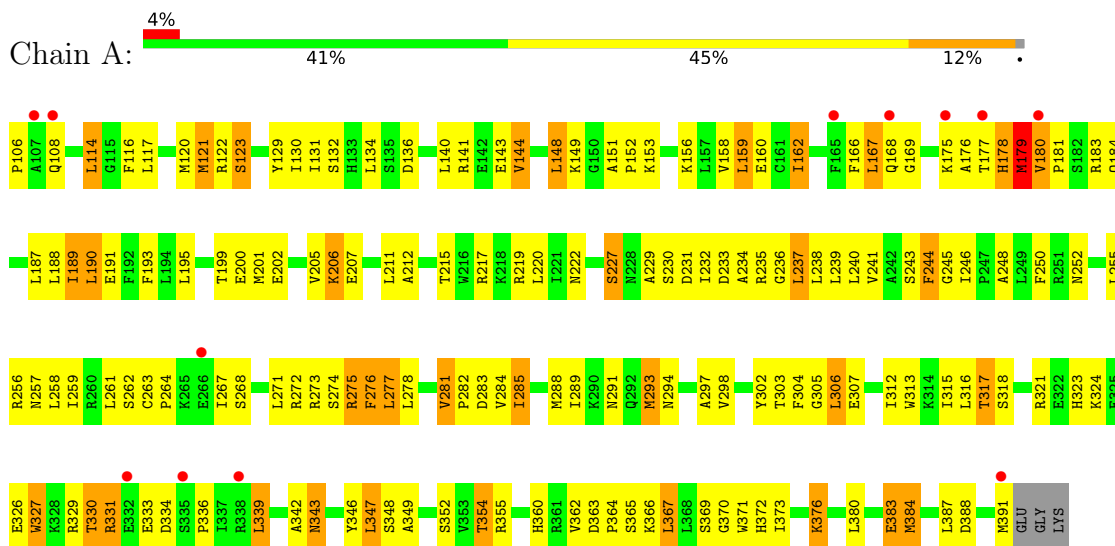
- Molecule 1 is a protein called FRIGIDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2279	1449	403	413	14			
1	B	285	Total	C	N	O	S	0	0	0
			2273	1445	402	412	14			
1	C	284	Total	C	N	O	S	0	0	0
			2267	1442	401	410	14			

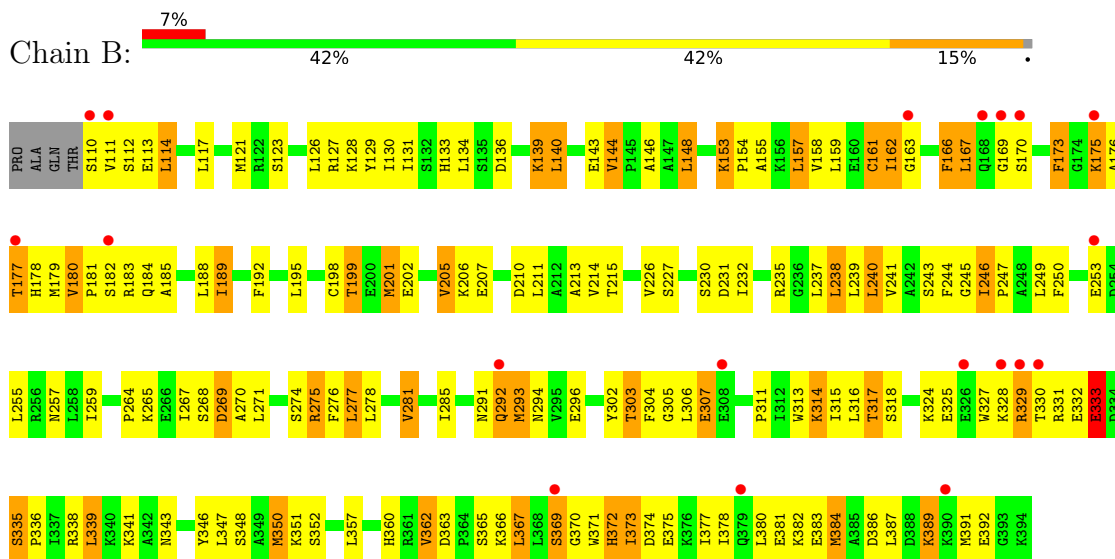
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FRIGIDA



• Molecule 1: FRIGIDA



• Molecule 1: FRIGIDA





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	148.88Å 148.88Å 262.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 3.26 46.96 – 3.26	Depositor EDS
% Data completeness (in resolution range)	86.7 (46.96-3.26) 86.8 (46.96-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 3.25Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.225 , 0.239 0.225 , 0.239	Depositor DCC
R_{free} test set	3661 reflections (8.43%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 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	0.94	EDS
Total number of atoms	6819	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	0.65	0/2319	1.06	10/3116 (0.3%)
1	B	0.75	3/2312 (0.1%)	1.16	14/3104 (0.5%)
1	C	0.65	0/2306	1.18	19/3096 (0.6%)
All	All	0.68	3/6937 (0.0%)	1.13	43/9316 (0.5%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	GLN	CD-OE1	11.72	1.45	1.23
1	B	292	GLN	CD-NE2	10.49	1.55	1.33
1	B	291	ASN	CG-ND2	5.35	1.44	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	GLY	N-CA-C	-13.25	91.91	112.45
1	B	182	SER	N-CA-C	-9.97	99.67	112.93
1	C	171	LYS	N-CA-C	8.39	121.64	109.14
1	C	151	ALA	CA-C-N	8.19	130.08	119.84
1	C	151	ALA	C-N-CA	8.19	130.08	119.84
1	C	200	GLU	N-CA-C	8.00	121.00	111.33
1	A	370	GLY	N-CA-C	-7.44	104.22	114.64
1	C	276	PHE	N-CA-C	-7.43	102.80	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	VAL	N-CA-C	-7.24	93.24	108.88
1	C	169	GLY	N-CA-C	7.23	123.25	113.99
1	C	153	LYS	CA-C-N	7.12	126.75	119.56
1	C	153	LYS	C-N-CA	7.12	126.75	119.56
1	C	393	GLY	N-CA-C	7.05	121.17	112.64
1	B	144	VAL	CB-CA-C	-6.95	106.98	114.35
1	B	291	ASN	CA-C-N	-6.76	112.48	122.41
1	B	291	ASN	C-N-CA	-6.76	112.48	122.41
1	A	276	PHE	N-CA-C	-6.67	103.49	111.69
1	C	312	ILE	N-CA-C	-6.58	105.41	111.67
1	B	291	ASN	CA-C-O	-6.49	113.34	120.81
1	A	334	ASP	N-CA-C	6.46	124.56	110.80
1	A	202	GLU	CA-C-N	6.36	126.85	119.47
1	A	202	GLU	C-N-CA	6.36	126.85	119.47
1	C	281	VAL	N-CA-CB	6.17	114.39	110.50
1	C	291	ASN	N-CA-C	6.06	120.38	112.92
1	B	246	ILE	N-CA-C	5.95	114.43	107.77
1	C	281	VAL	CB-CA-C	-5.89	108.11	114.35
1	B	153	LYS	CA-C-N	5.83	125.37	119.19
1	B	153	LYS	C-N-CA	5.83	125.37	119.19
1	B	179	MET	N-CA-C	5.83	118.02	108.52
1	C	310	PHE	CA-C-N	-5.70	112.71	119.84
1	C	310	PHE	C-N-CA	-5.70	112.71	119.84
1	C	246	ILE	N-CA-C	5.57	113.38	107.76
1	C	231	ASP	N-CA-C	-5.53	104.27	111.02
1	C	143	GLU	N-CA-C	5.40	119.93	113.23
1	A	144	VAL	CA-C-N	-5.35	113.11	119.05
1	A	144	VAL	C-N-CA	-5.35	113.11	119.05
1	B	173	PHE	N-CA-C	5.28	122.05	110.80
1	B	333	GLU	N-CA-C	5.18	117.06	108.20
1	B	268	SER	N-CA-C	5.17	117.33	111.02
1	A	143	GLU	N-CA-C	5.11	117.63	111.40
1	B	329	ARG	N-CA-C	-5.09	104.82	111.02
1	A	383	GLU	N-CA-C	5.04	117.51	111.71
1	C	201	MET	N-CA-C	5.02	117.63	110.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	MET	Peptide
1	A	333	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	369	SER	Peptide

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	2279	0	2352	178	0
1	B	2273	0	2346	180	0
1	C	2267	0	2341	181	0
All	All	6819	0	7039	526	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 38.

All (526) 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:A:331:ARG:HG3	1:A:331:ARG:HH11	1.08	1.12
1:C:274:SER:O	1:C:275:ARG:HB3	1.60	1.02
1:C:355:ARG:HH11	1:C:355:ARG:HG2	1.22	1.01
1:B:281:VAL:HG21	1:B:304:PHE:CE2	1.95	0.99
1:A:211:LEU:HD22	1:B:347:LEU:HD13	1.43	0.98
1:B:188:LEU:HD12	1:B:192:PHE:CZ	1.98	0.98
1:A:179:MET:HG3	1:A:181:PRO:HA	1.43	0.98
1:C:172:ALA:HB3	1:C:175:LYS:HB2	1.46	0.98
1:B:267:ILE:HG22	1:B:271:LEU:HG	1.46	0.96
1:A:162:ILE:HD11	1:A:190:LEU:HD23	1.48	0.93
1:B:114:LEU:HG	1:B:129:TYR:CE1	2.05	0.91
1:C:280:ARG:CG	1:C:280:ARG:HH11	1.84	0.90
1:A:365:SER:O	1:A:369:SER:N	2.04	0.89
1:B:247:PRO:HG2	1:B:250:PHE:CD1	2.08	0.88
1:C:280:ARG:HH11	1:C:280:ARG:HG3	1.37	0.88
1:A:331:ARG:HG3	1:A:331:ARG:NH1	1.88	0.88
1:A:162:ILE:HD11	1:A:190:LEU:CD2	2.04	0.87
1:B:372:HIS:HB3	1:B:375:GLU:HG3	1.56	0.87
1:A:331:ARG:HH11	1:A:331:ARG:CG	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:THR:HG22	1:B:304:PHE:HD1	1.38	0.86
1:B:114:LEU:HG	1:B:129:TYR:HE1	1.36	0.86
1:B:121:MET:CE	1:B:153:LYS:H	1.87	0.86
1:A:179:MET:O	1:A:179:MET:HG2	1.73	0.86
1:A:347:LEU:HD13	1:C:211:LEU:HG	1.56	0.86
1:B:303:THR:HG22	1:B:304:PHE:CD1	2.11	0.86
1:A:258:LEU:O	1:A:262:SER:HB2	1.75	0.86
1:A:141:ARG:NH1	1:A:191:GLU:OE2	2.10	0.85
1:C:166:PHE:O	1:C:219:ARG:NH2	2.10	0.85
1:C:172:ALA:HB2	1:C:183:ARG:HH22	1.39	0.85
1:B:267:ILE:CG2	1:B:271:LEU:HG	2.07	0.84
1:A:177:THR:C	1:A:179:MET:H	1.84	0.84
1:C:118:CYS:HB3	1:C:151:ALA:HB2	1.56	0.84
1:C:120:MET:HA	1:C:120:MET:HE2	1.58	0.84
1:B:302:TYR:HB3	1:B:360:HIS:ND1	1.94	0.83
1:B:188:LEU:HD12	1:B:192:PHE:HZ	1.43	0.82
1:A:330:THR:HG21	1:A:342:ALA:HB2	1.62	0.82
1:A:230:SER:HB2	1:A:233:ASP:H	1.41	0.82
1:C:302:TYR:CE2	1:C:307:GLU:HG2	2.14	0.81
1:C:171:LYS:HG3	1:C:175:LYS:HE2	1.63	0.80
1:B:357:LEU:HD22	1:B:362:VAL:HG11	1.64	0.80
1:B:158:VAL:HG13	1:B:189:ILE:HG22	1.64	0.79
1:A:363:ASP:HB3	1:A:366:LYS:HG3	1.65	0.79
1:C:339:LEU:HB3	1:C:387:LEU:HD11	1.63	0.79
1:A:134:LEU:HD13	1:A:179:MET:CE	2.12	0.79
1:B:281:VAL:HG21	1:B:304:PHE:HE2	1.45	0.78
1:A:339:LEU:HD12	1:A:387:LEU:HD21	1.64	0.78
1:B:155:ALA:HB2	1:B:201:MET:HB3	1.63	0.78
1:C:127:ARG:O	1:C:131:ILE:HG13	1.82	0.78
1:B:129:TYR:HE2	1:B:133:HIS:CD2	2.03	0.77
1:B:372:HIS:CB	1:B:375:GLU:HG3	2.15	0.77
1:A:238:LEU:CD1	1:A:271:LEU:HD21	2.14	0.77
1:B:158:VAL:HG13	1:B:189:ILE:CG2	2.14	0.77
1:A:331:ARG:HD2	1:A:331:ARG:N	1.99	0.76
1:C:324:LYS:HE3	1:C:346:TYR:OH	1.86	0.76
1:B:367:LEU:HD22	1:B:367:LEU:O	1.87	0.75
1:B:155:ALA:CB	1:B:201:MET:HB3	2.16	0.74
1:C:157:LEU:O	1:C:161:CYS:HB2	1.86	0.74
1:B:167:LEU:HD23	1:B:167:LEU:H	1.51	0.73
1:B:185:ALA:O	1:B:189:ILE:HD12	1.87	0.73
1:B:201:MET:CE	1:B:206:LYS:HD2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:VAL:HG22	1:C:246:ILE:HA	1.70	0.73
1:B:199:THR:HG22	1:B:275:ARG:NH2	2.04	0.72
1:C:232:ILE:HD12	1:C:232:ILE:H	1.54	0.72
1:C:311:PRO:O	1:C:315:ILE:HG13	1.88	0.72
1:C:355:ARG:HG2	1:C:355:ARG:NH1	1.97	0.72
1:B:255:LEU:O	1:B:259:ILE:HG13	1.90	0.72
1:B:363:ASP:HB3	1:B:366:LYS:HG2	1.72	0.71
1:A:355:ARG:HH12	1:C:164:ARG:HH11	1.38	0.71
1:B:302:TYR:CD2	1:B:307:GLU:HG2	2.25	0.71
1:B:127:ARG:O	1:B:131:ILE:HG13	1.90	0.71
1:A:330:THR:C	1:A:331:ARG:HD2	2.16	0.70
1:C:302:TYR:CD2	1:C:307:GLU:HG2	2.26	0.70
1:B:144:VAL:HG12	1:B:148:LEU:HD12	1.72	0.70
1:A:134:LEU:HD13	1:A:179:MET:HE1	1.74	0.69
1:A:302:TYR:HB3	1:A:360:HIS:CD2	2.27	0.69
1:C:281:VAL:HA	1:C:284:VAL:HG13	1.74	0.69
1:C:193:PHE:CE2	1:C:243:SER:HB3	2.27	0.69
1:B:302:TYR:CE2	1:B:307:GLU:HG2	2.27	0.69
1:A:302:TYR:CB	1:A:360:HIS:CD2	2.76	0.69
1:A:312:ILE:HG21	1:A:367:LEU:HD11	1.73	0.69
1:A:323:HIS:ND1	1:A:349:ALA:CB	2.56	0.68
1:B:110:SER:HB3	1:B:143:GLU:OE2	1.92	0.68
1:B:339:LEU:HB3	1:B:387:LEU:HD21	1.75	0.68
1:C:255:LEU:O	1:C:259:ILE:HG13	1.94	0.68
1:C:267:ILE:HG22	1:C:271:LEU:HD12	1.76	0.68
1:A:365:SER:O	1:A:369:SER:HB2	1.94	0.68
1:C:311:PRO:HB2	1:C:314:LYS:HB2	1.76	0.67
1:A:343:ASN:HB3	1:A:384:MET:SD	2.34	0.67
1:C:362:VAL:O	1:C:364:PRO:HD3	1.95	0.67
1:A:274:SER:O	1:A:275:ARG:HB3	1.95	0.66
1:B:253:GLU:O	1:B:257:ASN:ND2	2.28	0.66
1:B:331:ARG:HG3	1:B:332:GLU:HG2	1.76	0.66
1:C:149:LYS:HE2	1:C:196:SER:O	1.95	0.66
1:C:210:ASP:O	1:C:214:VAL:HG23	1.96	0.66
1:C:171:LYS:HE3	1:C:175:LYS:HE2	1.77	0.66
1:B:350:MET:HE3	1:B:377:ILE:HG13	1.78	0.66
1:C:162:ILE:CG2	1:C:163:GLY:H	2.08	0.66
1:C:172:ALA:HB3	1:C:175:LYS:CB	2.25	0.66
1:C:156:LYS:HB3	1:C:205:VAL:CG2	2.26	0.65
1:B:365:SER:O	1:B:369:SER:HB2	1.96	0.65
1:B:154:PRO:O	1:B:158:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:THR:O	1:C:358:GLU:HG2	1.95	0.65
1:B:339:LEU:HD12	1:B:387:LEU:HD21	1.78	0.64
1:A:176:ALA:C	1:A:178:HIS:H	2.03	0.64
1:B:201:MET:HE3	1:B:206:LYS:HD2	1.79	0.64
1:B:331:ARG:NH2	1:B:339:LEU:HD21	2.13	0.64
1:C:193:PHE:HE2	1:C:243:SER:HB3	1.63	0.64
1:C:162:ILE:CG2	1:C:163:GLY:N	2.60	0.64
1:C:259:ILE:O	1:C:264:PRO:HG3	1.97	0.64
1:A:177:THR:C	1:A:179:MET:N	2.51	0.64
1:B:336:PRO:HB2	1:B:391:MET:HG3	1.78	0.64
1:C:137:VAL:HA	1:C:140:LEU:HD12	1.79	0.63
1:C:267:ILE:CG2	1:C:271:LEU:HG	2.28	0.63
1:A:365:SER:C	1:A:369:SER:HB2	2.24	0.63
1:A:321:ARG:HG3	1:A:371:TRP:HZ2	1.64	0.63
1:B:114:LEU:CG	1:B:129:TYR:CE1	2.81	0.63
1:B:235:ARG:HD3	1:B:267:ILE:HD11	1.79	0.63
1:A:241:VAL:HG11	1:A:246:ILE:HG12	1.81	0.63
1:A:131:ILE:HA	1:A:134:LEU:HD12	1.81	0.62
1:B:114:LEU:CG	1:B:129:TYR:HE1	2.12	0.62
1:B:277:LEU:O	1:B:281:VAL:HB	2.00	0.62
1:C:139:LYS:O	1:C:143:GLU:HG2	1.99	0.62
1:C:198:CYS:HB3	1:C:200:GLU:HG2	1.81	0.62
1:C:357:LEU:HD22	1:C:362:VAL:HG11	1.80	0.62
1:A:177:THR:O	1:A:179:MET:N	2.33	0.62
1:A:326:GLU:HA	1:A:329:ARG:HD2	1.81	0.62
1:C:156:LYS:HB3	1:C:205:VAL:HG22	1.81	0.62
1:B:235:ARG:CD	1:B:267:ILE:HD11	2.30	0.62
1:C:162:ILE:HG23	1:C:163:GLY:N	2.15	0.62
1:A:257:ASN:O	1:A:261:LEU:HB2	1.99	0.61
1:A:304:PHE:O	1:A:306:LEU:HD23	2.01	0.61
1:A:179:MET:O	1:A:179:MET:CG	2.47	0.61
1:A:259:ILE:O	1:A:264:PRO:CG	2.49	0.61
1:B:176:ALA:C	1:B:178:HIS:H	2.08	0.61
1:A:263:CYS:N	1:A:264:PRO:HD3	2.15	0.61
1:B:311:PRO:O	1:B:315:ILE:HG13	2.00	0.61
1:C:167:LEU:HD13	1:C:212:ALA:HA	1.83	0.60
1:C:354:THR:HG22	1:C:355:ARG:HD3	1.83	0.60
1:A:327:TRP:O	1:A:331:ARG:HD3	2.01	0.60
1:B:324:LYS:O	1:B:327:TRP:HB3	2.01	0.60
1:C:172:ALA:HB2	1:C:183:ARG:NH2	2.14	0.60
1:A:241:VAL:CG1	1:A:246:ILE:HG12	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:HD23	1:A:306:LEU:N	2.15	0.60
1:A:323:HIS:ND1	1:A:349:ALA:HB2	2.16	0.60
1:B:336:PRO:CB	1:B:391:MET:HG3	2.32	0.60
1:B:374:ASP:O	1:B:378:ILE:HG12	2.02	0.60
1:C:306:LEU:HD23	1:C:306:LEU:N	2.17	0.60
1:C:267:ILE:HG22	1:C:271:LEU:CD1	2.32	0.59
1:A:252:ASN:HB3	1:A:284:VAL:HG22	1.84	0.59
1:B:339:LEU:CD1	1:B:387:LEU:HD21	2.32	0.59
1:C:130:ILE:HG23	1:C:140:LEU:HD22	1.85	0.59
1:B:130:ILE:HD12	1:B:189:ILE:HD11	1.85	0.59
1:B:129:TYR:C	1:B:129:TYR:CD2	2.80	0.59
1:B:339:LEU:HB3	1:B:387:LEU:CD2	2.32	0.59
1:C:281:VAL:O	1:C:285:ILE:HG13	2.02	0.59
1:A:274:SER:CB	1:A:277:LEU:HB2	2.33	0.58
1:C:119:GLY:HA2	1:C:152:PRO:HD3	1.84	0.58
1:A:121:MET:HE3	1:A:153:LYS:H	1.67	0.58
1:A:336:PRO:HB2	1:A:391:MET:SD	2.43	0.58
1:C:275:ARG:O	1:C:275:ARG:HG2	2.03	0.58
1:B:175:LYS:O	1:B:176:ALA:HB3	2.03	0.57
1:C:280:ARG:CG	1:C:280:ARG:NH1	2.54	0.57
1:A:238:LEU:HD11	1:A:271:LEU:HD21	1.85	0.57
1:B:121:MET:HE2	1:B:153:LYS:H	1.65	0.57
1:C:216:TRP:CD1	1:C:220:LEU:HD12	2.39	0.57
1:C:171:LYS:HD2	1:C:175:LYS:HG3	1.85	0.57
1:B:129:TYR:CE2	1:B:133:HIS:CE1	2.93	0.57
1:B:274:SER:OG	1:B:275:ARG:N	2.36	0.56
1:C:171:LYS:HE3	1:C:175:LYS:CE	2.34	0.56
1:A:201:MET:SD	1:A:206:LYS:HG3	2.45	0.56
1:C:232:ILE:HD12	1:C:232:ILE:N	2.19	0.56
1:C:349:ALA:O	1:C:352:SER:HB3	2.05	0.56
1:A:346:TYR:OH	1:A:376:LYS:HE3	2.06	0.56
1:C:284:VAL:O	1:C:288:MET:HG3	2.05	0.56
1:B:247:PRO:HG2	1:B:250:PHE:CE1	2.41	0.56
1:A:298:VAL:HG23	1:A:315:ILE:HG21	1.87	0.56
1:A:215:THR:HG22	1:B:348:SER:OG	2.06	0.56
1:B:143:GLU:O	1:B:146:ALA:HB3	2.06	0.56
1:B:311:PRO:HB2	1:B:314:LYS:HB2	1.87	0.56
1:C:213:ALA:HB2	1:C:240:LEU:HD13	1.87	0.56
1:A:121:MET:CE	1:A:153:LYS:H	2.20	0.56
1:A:323:HIS:O	1:A:346:TYR:CD1	2.59	0.55
1:A:237:LEU:HD13	1:A:258:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:MET:O	1:A:388:ASP:HB2	2.06	0.55
1:B:130:ILE:HD12	1:B:189:ILE:CD1	2.37	0.55
1:C:216:TRP:HD1	1:C:220:LEU:HD12	1.71	0.55
1:B:129:TYR:HE2	1:B:133:HIS:CG	2.24	0.55
1:B:167:LEU:HD23	1:B:167:LEU:N	2.20	0.55
1:B:274:SER:O	1:B:275:ARG:CB	2.55	0.55
1:C:165:PHE:HD2	1:C:165:PHE:N	2.04	0.55
1:C:165:PHE:N	1:C:165:PHE:CD2	2.75	0.55
1:A:121:MET:HE1	1:A:153:LYS:O	2.07	0.55
1:B:214:VAL:HG13	1:B:249:LEU:HD12	1.89	0.54
1:A:190:LEU:HD11	1:A:240:LEU:HA	1.88	0.54
1:A:324:LYS:HA	1:A:346:TYR:CE1	2.41	0.54
1:B:275:ARG:HA	1:B:278:LEU:HB2	1.89	0.54
1:B:346:TYR:HD2	1:B:380:LEU:HD11	1.72	0.54
1:C:216:TRP:CD1	1:C:220:LEU:CD1	2.90	0.54
1:A:331:ARG:NH2	1:A:383:GLU:OE2	2.36	0.54
1:B:134:LEU:CD1	1:B:181:PRO:HB3	2.37	0.54
1:B:331:ARG:CG	1:B:332:GLU:HG2	2.37	0.54
1:B:199:THR:HG22	1:B:275:ARG:HH21	1.73	0.54
1:A:244:PHE:CD1	1:A:244:PHE:N	2.75	0.54
1:A:298:VAL:HG21	1:A:316:LEU:HD21	1.87	0.54
1:A:158:VAL:HG23	1:A:244:PHE:HZ	1.72	0.54
1:A:291:ASN:HB3	1:A:293:MET:HG3	1.90	0.54
1:A:298:VAL:HG21	1:A:316:LEU:CD2	2.37	0.54
1:C:201:MET:CE	1:C:206:LYS:HD2	2.38	0.54
1:C:328:LYS:O	1:C:331:ARG:HB2	2.08	0.54
1:A:162:ILE:HD11	1:A:190:LEU:HD21	1.88	0.54
1:C:131:ILE:HG12	1:C:185:ALA:HB2	1.90	0.54
1:A:271:LEU:HD22	1:A:277:LEU:HD23	1.90	0.53
1:B:166:PHE:CE1	1:B:183:ARG:HG2	2.43	0.53
1:C:144:VAL:HG12	1:C:148:LEU:HD12	1.90	0.53
1:C:235:ARG:O	1:C:235:ARG:HG3	2.05	0.53
1:C:281:VAL:N	1:C:282:PRO:CD	2.71	0.53
1:C:298:VAL:HG21	1:C:316:LEU:HD21	1.90	0.53
1:C:144:VAL:N	1:C:145:PRO:HD2	2.24	0.53
1:C:173:PHE:C	1:C:175:LYS:H	2.17	0.53
1:C:179:MET:HE1	1:C:184:GLN:OE1	2.08	0.53
1:C:305:GLY:C	1:C:306:LEU:HD23	2.34	0.53
1:C:120:MET:HA	1:C:120:MET:CE	2.35	0.53
1:C:281:VAL:HA	1:C:284:VAL:CG1	2.37	0.53
1:B:169:GLY:O	1:B:170:SER:OG	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:SER:HB3	1:B:183:ARG:NH1	2.23	0.53
1:A:285:ILE:O	1:A:289:ILE:HG12	2.09	0.53
1:C:222:ASN:C	1:C:224:GLY:H	2.16	0.53
1:C:184:GLN:HG3	1:C:188:LEU:HD12	1.91	0.53
1:B:267:ILE:HG22	1:B:271:LEU:CG	2.30	0.52
1:B:274:SER:O	1:B:275:ARG:HB3	2.09	0.52
1:C:162:ILE:HG22	1:C:163:GLY:H	1.74	0.52
1:B:175:LYS:HB3	1:C:177:THR:HB	1.91	0.52
1:B:211:LEU:C	1:B:211:LEU:HD23	2.35	0.52
1:C:371:TRP:O	1:C:376:LYS:NZ	2.41	0.52
1:B:114:LEU:CD1	1:B:129:TYR:CE1	2.92	0.52
1:B:126:LEU:O	1:B:130:ILE:HG13	2.10	0.52
1:B:383:GLU:O	1:B:386:ASP:HB2	2.09	0.52
1:A:248:ALA:HB1	1:B:341:LYS:HG3	1.91	0.52
1:A:323:HIS:CE1	1:A:349:ALA:HB2	2.44	0.52
1:B:201:MET:HE1	1:B:206:LYS:HD2	1.89	0.52
1:B:176:ALA:O	1:B:178:HIS:N	2.42	0.52
1:C:246:ILE:HD13	1:C:255:LEU:HD21	1.92	0.52
1:C:298:VAL:HG21	1:C:316:LEU:CD2	2.39	0.52
1:B:305:GLY:C	1:B:306:LEU:HD23	2.35	0.52
1:A:307:GLU:HB2	1:A:312:ILE:HD11	1.92	0.52
1:A:339:LEU:O	1:A:343:ASN:HB2	2.09	0.52
1:A:178:HIS:O	1:A:179:MET:HB3	2.09	0.52
1:A:227:SER:O	1:A:261:LEU:HD11	2.10	0.52
1:A:245:GLY:HA2	1:A:276:PHE:CG	2.44	0.52
1:A:312:ILE:CG2	1:A:367:LEU:HD11	2.40	0.52
1:A:256:ARG:HA	1:A:259:ILE:HD12	1.91	0.51
1:C:151:ALA:HB1	1:C:152:PRO:HD2	1.92	0.51
1:B:170:SER:HB3	1:B:183:ARG:CZ	2.40	0.51
1:A:121:MET:HG3	1:A:152:PRO:HG2	1.92	0.51
1:B:269:ASP:OD2	1:B:269:ASP:N	2.43	0.51
1:C:281:VAL:O	1:C:284:VAL:HG13	2.10	0.51
1:C:346:TYR:CD2	1:C:380:LEU:HD11	2.45	0.51
1:A:275:ARG:HA	1:A:278:LEU:HB2	1.93	0.51
1:B:335:SER:HB3	1:B:338:ARG:HB2	1.92	0.51
1:C:280:ARG:HG3	1:C:280:ARG:NH1	2.17	0.51
1:B:372:HIS:ND1	1:B:372:HIS:N	2.57	0.51
1:A:274:SER:HB3	1:A:277:LEU:HB2	1.93	0.51
1:A:114:LEU:HG	1:A:129:TYR:CE2	2.46	0.50
1:A:176:ALA:C	1:A:178:HIS:N	2.68	0.50
1:A:272:ARG:HE	1:A:305:GLY:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ALA:HB1	1:B:205:VAL:HG21	1.92	0.50
1:A:275:ARG:O	1:A:275:ARG:HG2	2.10	0.50
1:A:355:ARG:NH1	1:C:164:ARG:HH11	2.08	0.50
1:B:389:LYS:HB2	1:B:389:LYS:NZ	2.26	0.50
1:C:171:LYS:HE3	1:C:175:LYS:NZ	2.25	0.50
1:C:180:VAL:HG13	1:C:183:ARG:HG2	1.92	0.50
1:C:175:LYS:HG2	1:C:176:ALA:N	2.27	0.50
1:A:321:ARG:HG3	1:A:371:TRP:CZ2	2.47	0.50
1:B:162:ILE:HG12	1:B:163:GLY:N	2.26	0.50
1:C:180:VAL:HG22	1:C:182:SER:H	1.75	0.50
1:A:187:LEU:HD21	1:A:236:GLY:HA2	1.93	0.50
1:C:178:HIS:O	1:C:179:MET:HB2	2.12	0.50
1:C:241:VAL:CG2	1:C:247:PRO:HD2	2.41	0.50
1:C:350:MET:HG2	1:C:373:ILE:HG23	1.94	0.50
1:C:367:LEU:O	1:C:367:LEU:HD22	2.12	0.50
1:B:129:TYR:HE2	1:B:133:HIS:NE2	2.09	0.50
1:B:246:ILE:HD13	1:B:255:LEU:HD21	1.94	0.50
1:A:179:MET:HE2	1:A:181:PRO:HB3	1.93	0.49
1:B:121:MET:HE1	1:B:153:LYS:O	2.11	0.49
1:B:129:TYR:C	1:B:129:TYR:HD2	2.20	0.49
1:C:153:LYS:HE2	1:C:153:LYS:N	2.26	0.49
1:C:157:LEU:O	1:C:157:LEU:HD23	2.12	0.49
1:C:156:LYS:HB3	1:C:205:VAL:HG21	1.94	0.49
1:A:114:LEU:HD11	1:A:144:VAL:HG22	1.93	0.49
1:B:346:TYR:CD2	1:B:380:LEU:HD11	2.48	0.49
1:A:229:ALA:HB3	1:A:261:LEU:HD13	1.94	0.49
1:A:193:PHE:CE2	1:A:243:SER:HB3	2.48	0.49
1:A:123:SER:HB3	1:A:160:GLU:HB3	1.94	0.48
1:A:302:TYR:HB2	1:A:360:HIS:CD2	2.48	0.48
1:A:347:LEU:HD13	1:C:211:LEU:CG	2.36	0.48
1:B:184:GLN:HG2	1:B:188:LEU:HD23	1.94	0.48
1:A:190:LEU:CD1	1:A:240:LEU:HA	2.43	0.48
1:B:136:ASP:OD1	1:B:139:LYS:HB2	2.13	0.48
1:C:117:LEU:CD1	1:C:122:ARG:HB2	2.43	0.48
1:A:106:PRO:HB2	1:A:108:GLN:HG2	1.96	0.48
1:B:371:TRP:O	1:B:372:HIS:C	2.54	0.48
1:A:255:LEU:O	1:A:259:ILE:HG13	2.14	0.48
1:C:141:ARG:NH2	1:C:191:GLU:OE1	2.45	0.48
1:C:165:PHE:HA	1:C:168:GLN:HB3	1.94	0.48
1:B:111:VAL:O	1:B:111:VAL:HG22	2.13	0.48
1:A:121:MET:HG3	1:A:152:PRO:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:HD13	1:B:271:LEU:HD21	1.95	0.48
1:B:372:HIS:HB2	1:B:375:GLU:HG3	1.95	0.48
1:C:157:LEU:HD23	1:C:157:LEU:C	2.39	0.48
1:C:167:LEU:HD23	1:C:167:LEU:H	1.79	0.48
1:A:193:PHE:HE2	1:A:243:SER:HB3	1.78	0.48
1:B:175:LYS:HD2	1:B:175:LYS:HA	1.73	0.48
1:B:371:TRP:O	1:B:373:ILE:HG12	2.13	0.48
1:C:232:ILE:H	1:C:232:ILE:CD1	2.24	0.48
1:A:190:LEU:HD12	1:A:239:LEU:C	2.38	0.48
1:A:207:GLU:OE1	1:B:384:MET:HE3	2.13	0.48
1:A:158:VAL:HG11	1:A:193:PHE:HB2	1.95	0.47
1:B:241:VAL:HB	1:B:246:ILE:HG12	1.95	0.47
1:C:355:ARG:HH11	1:C:355:ARG:CG	2.09	0.47
1:C:211:LEU:HD13	1:C:215:THR:HG23	1.96	0.47
1:C:355:ARG:HD3	1:C:355:ARG:N	2.29	0.47
1:C:374:ASP:O	1:C:378:ILE:HG12	2.14	0.47
1:A:343:ASN:ND2	1:A:380:LEU:HD22	2.29	0.47
1:B:157:LEU:HD23	1:B:157:LEU:O	2.14	0.47
1:B:166:PHE:HB3	1:B:167:LEU:HD23	1.95	0.47
1:B:357:LEU:HD22	1:B:362:VAL:CG1	2.39	0.47
1:A:323:HIS:O	1:A:346:TYR:HD1	1.97	0.47
1:C:116:PHE:O	1:C:120:MET:HB2	2.14	0.47
1:C:355:ARG:O	1:C:356:CYS:C	2.58	0.47
1:C:241:VAL:O	1:C:245:GLY:N	2.48	0.47
1:B:350:MET:HB2	1:B:350:MET:HE2	1.70	0.47
1:B:367:LEU:HD22	1:B:367:LEU:C	2.35	0.47
1:C:195:LEU:HD23	1:C:270:ALA:HB2	1.96	0.47
1:B:350:MET:HG2	1:B:373:ILE:HG23	1.97	0.47
1:C:162:ILE:HD11	1:C:190:LEU:HG	1.96	0.47
1:A:302:TYR:CE1	1:A:312:ILE:HD13	2.50	0.46
1:B:180:VAL:HG13	1:B:181:PRO:CD	2.45	0.46
1:C:389:LYS:HB2	1:C:389:LYS:HE3	1.60	0.46
1:A:201:MET:CE	1:A:205:VAL:HG12	2.45	0.46
1:A:330:THR:CG2	1:A:342:ALA:HB2	2.39	0.46
1:B:121:MET:HE1	1:B:153:LYS:C	2.40	0.46
1:C:271:LEU:HD22	1:C:277:LEU:CD2	2.45	0.46
1:C:274:SER:OG	1:C:277:LEU:HB2	2.15	0.46
1:B:317:THR:HG22	1:B:318:SER:N	2.29	0.46
1:C:171:LYS:CG	1:C:175:LYS:HE2	2.41	0.46
1:A:149:LYS:HB3	1:A:149:LYS:HE3	1.69	0.46
1:A:272:ARG:HE	1:A:304:PHE:C	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD12	1:B:129:TYR:HD1	1.79	0.46
1:B:157:LEU:O	1:B:161:CYS:HB2	2.14	0.46
1:C:281:VAL:CA	1:C:284:VAL:HG13	2.43	0.46
1:A:363:ASP:HB3	1:A:366:LYS:CG	2.41	0.46
1:C:334:ASP:O	1:C:335:SER:C	2.57	0.46
1:A:234:ALA:HA	1:A:258:LEU:CD2	2.45	0.46
1:C:288:MET:O	1:C:293:MET:HB2	2.15	0.46
1:A:201:MET:HE1	1:A:205:VAL:HG12	1.97	0.46
1:B:129:TYR:HD2	1:B:129:TYR:O	1.98	0.46
1:B:306:LEU:HD23	1:B:306:LEU:N	2.31	0.46
1:B:302:TYR:CZ	1:B:362:VAL:HG21	2.51	0.46
1:B:328:LYS:O	1:B:329:ARG:C	2.59	0.46
1:C:158:VAL:HG21	1:C:193:PHE:HB2	1.98	0.46
1:A:187:LEU:HD21	1:A:236:GLY:CA	2.46	0.46
1:A:232:ILE:HD13	1:C:173:PHE:CE2	2.50	0.46
1:A:268:SER:HA	1:A:271:LEU:HB2	1.97	0.46
1:C:267:ILE:HG23	1:C:271:LEU:HG	1.97	0.46
1:A:167:LEU:HD13	1:A:212:ALA:CB	2.46	0.46
1:B:176:ALA:C	1:B:178:HIS:N	2.73	0.46
1:A:175:LYS:HD3	1:A:180:VAL:HG22	1.97	0.45
1:A:343:ASN:HD22	1:A:384:MET:HG2	1.81	0.45
1:C:198:CYS:CB	1:C:200:GLU:HG2	2.46	0.45
1:B:207:GLU:OE1	1:C:384:MET:HE3	2.17	0.45
1:A:130:ILE:HD13	1:A:189:ILE:HG12	1.98	0.45
1:B:129:TYR:CE2	1:B:133:HIS:NE2	2.85	0.45
1:B:183:ARG:O	1:B:184:GLN:C	2.59	0.45
1:C:268:SER:O	1:C:269:ASP:C	2.58	0.45
1:C:337:ILE:HG22	1:C:341:LYS:HE2	1.98	0.45
1:A:347:LEU:HD23	1:A:347:LEU:HA	1.74	0.45
1:C:211:LEU:HD22	1:C:211:LEU:HA	1.65	0.45
1:A:281:VAL:HG12	1:A:282:PRO:HD3	1.99	0.45
1:C:238:LEU:HD13	1:C:271:LEU:HD21	1.99	0.45
1:A:167:LEU:HD13	1:A:212:ALA:HB1	1.98	0.45
1:A:241:VAL:HG21	1:A:250:PHE:CE1	2.52	0.45
1:C:152:PRO:O	1:C:153:LYS:HB2	2.17	0.45
1:C:313:TRP:HD1	1:C:367:LEU:HD22	1.81	0.45
1:A:271:LEU:HD22	1:A:277:LEU:CD2	2.47	0.45
1:C:257:ASN:OD1	1:C:260:ARG:NH2	2.47	0.45
1:A:272:ARG:O	1:A:278:LEU:HD11	2.16	0.45
1:A:166:PHE:CE1	1:A:183:ARG:NH1	2.85	0.45
1:B:175:LYS:HB2	1:C:231:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HE2	1:C:139:LYS:HB3	1.62	0.45
1:C:241:VAL:HG21	1:C:250:PHE:CE2	2.51	0.45
1:A:116:PHE:CD2	1:A:116:PHE:C	2.95	0.44
1:B:294:ASN:HB3	1:B:315:ILE:HG22	1.98	0.44
1:C:332:GLU:OE1	1:C:332:GLU:HA	2.17	0.44
1:A:116:PHE:CZ	1:A:120:MET:HG3	2.52	0.44
1:B:357:LEU:HA	1:B:357:LEU:HD23	1.66	0.44
1:A:195:LEU:HA	1:A:273:ARG:NH1	2.31	0.44
1:A:317:THR:O	1:A:318:SER:C	2.61	0.44
1:C:157:LEU:C	1:C:157:LEU:CD2	2.91	0.44
1:B:386:ASP:O	1:B:389:LYS:HG2	2.17	0.44
1:A:365:SER:O	1:A:366:LYS:C	2.61	0.44
1:B:259:ILE:O	1:B:264:PRO:HG3	2.18	0.44
1:C:144:VAL:HG11	1:C:192:PHE:CD1	2.52	0.44
1:C:258:LEU:HD23	1:C:258:LEU:HA	1.56	0.44
1:A:114:LEU:HD11	1:A:144:VAL:CG2	2.48	0.44
1:A:302:TYR:CE1	1:A:312:ILE:CD1	3.00	0.44
1:B:130:ILE:HD12	1:B:189:ILE:HG13	2.00	0.44
1:B:134:LEU:HD11	1:B:181:PRO:HB3	1.99	0.44
1:B:267:ILE:HG22	1:B:267:ILE:O	2.18	0.44
1:B:339:LEU:HD23	1:B:339:LEU:HA	1.64	0.44
1:B:347:LEU:HD11	1:B:381:GLU:HG2	1.99	0.44
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.78	0.44
1:C:331:ARG:HD2	1:C:331:ARG:HA	1.70	0.44
1:A:121:MET:HE1	1:A:153:LYS:C	2.42	0.44
1:B:213:ALA:HB2	1:B:240:LEU:HD13	1.99	0.44
1:B:304:PHE:HD1	1:B:304:PHE:N	2.16	0.44
1:B:140:LEU:O	1:B:144:VAL:HG23	2.18	0.44
1:B:293:MET:HE2	1:B:296:GLU:OE1	2.18	0.44
1:B:293:MET:O	1:B:294:ASN:C	2.61	0.43
1:C:296:GLU:OE1	1:C:296:GLU:N	2.44	0.43
1:C:336:PRO:HG2	1:C:337:ILE:CD1	2.48	0.43
1:B:304:PHE:CD1	1:B:304:PHE:N	2.86	0.43
1:C:195:LEU:HD12	1:C:195:LEU:O	2.17	0.43
1:A:313:TRP:O	1:A:317:THR:HB	2.18	0.43
1:A:134:LEU:HD13	1:A:179:MET:HE3	1.95	0.43
1:A:362:VAL:HG11	1:A:367:LEU:HD12	2.01	0.43
1:B:245:GLY:HA2	1:B:276:PHE:CD2	2.53	0.43
1:C:118:CYS:SG	1:C:147:ALA:HB1	2.58	0.43
1:A:176:ALA:O	1:A:178:HIS:N	2.52	0.43
1:C:217:ARG:O	1:C:221:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:O	1:C:144:VAL:HG23	2.18	0.43
1:A:201:MET:HE2	1:A:206:LYS:N	2.34	0.43
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.75	0.43
1:B:243:SER:HB2	1:B:244:PHE:CD1	2.54	0.43
1:B:294:ASN:ND2	1:B:294:ASN:H	2.16	0.43
1:C:169:GLY:O	1:C:170:SER:HB2	2.19	0.43
1:C:179:MET:HG2	1:C:232:ILE:HG12	2.01	0.43
1:C:291:ASN:O	1:C:292:GLN:HB2	2.18	0.43
1:B:302:TYR:OH	1:B:362:VAL:HG21	2.17	0.43
1:C:288:MET:HE3	1:C:288:MET:HB3	1.83	0.43
1:C:337:ILE:HD12	1:C:337:ILE:N	2.33	0.43
1:A:274:SER:O	1:A:275:ARG:CB	2.63	0.43
1:B:129:TYR:HE2	1:B:133:HIS:CE1	2.35	0.43
1:B:159:LEU:HA	1:B:159:LEU:HD23	1.48	0.43
1:B:303:THR:HG22	1:B:304:PHE:CE1	2.54	0.43
1:C:165:PHE:HZ	1:C:182:SER:HB2	1.84	0.43
1:B:140:LEU:HD23	1:B:144:VAL:CG2	2.49	0.43
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.69	0.42
1:A:189:ILE:HD13	1:A:189:ILE:HA	1.87	0.42
1:B:117:LEU:HD13	1:B:126:LEU:HA	2.01	0.42
1:B:134:LEU:HD12	1:B:181:PRO:HB3	2.01	0.42
1:B:166:PHE:CD1	1:B:183:ARG:HG2	2.54	0.42
1:C:161:CYS:SG	1:C:189:ILE:HD13	2.59	0.42
1:A:232:ILE:HD12	1:A:232:ILE:HG23	1.80	0.42
1:B:117:LEU:HD23	1:B:117:LEU:HA	1.69	0.42
1:B:325:GLU:O	1:B:328:LYS:N	2.51	0.42
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.79	0.42
1:B:128:LYS:HA	1:B:128:LYS:HD3	1.88	0.42
1:C:277:LEU:HD12	1:C:277:LEU:HA	1.80	0.42
1:C:357:LEU:HD22	1:C:362:VAL:CG1	2.47	0.42
1:A:354:THR:HG22	1:A:355:ARG:N	2.33	0.42
1:B:210:ASP:O	1:B:214:VAL:HG23	2.20	0.42
1:C:162:ILE:HA	1:C:162:ILE:HD12	1.65	0.42
1:C:320:LEU:HD11	1:C:368:LEU:HD13	2.01	0.42
1:B:347:LEU:HD11	1:B:381:GLU:CG	2.50	0.42
1:A:134:LEU:CD2	1:A:184:GLN:HG2	2.50	0.42
1:B:267:ILE:CG2	1:B:267:ILE:O	2.67	0.42
1:A:148:LEU:HD12	1:A:193:PHE:HA	2.01	0.42
1:B:112:SER:O	1:B:113:GLU:C	2.62	0.42
1:C:117:LEU:HD13	1:C:122:ARG:HB2	2.01	0.42
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ALA:HB2	1:C:240:LEU:CD1	2.49	0.42
1:C:118:CYS:CB	1:C:151:ALA:HB2	2.40	0.42
1:C:324:LYS:HE3	1:C:346:TYR:CZ	2.55	0.42
1:A:178:HIS:O	1:A:179:MET:CB	2.68	0.41
1:A:259:ILE:O	1:A:264:PRO:HG2	2.18	0.41
1:A:315:ILE:HG22	1:A:316:LEU:N	2.35	0.41
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.82	0.41
1:B:180:VAL:HG13	1:B:181:PRO:HD2	2.02	0.41
1:C:269:ASP:OD1	1:C:269:ASP:N	2.52	0.41
1:A:363:ASP:HA	1:A:364:PRO:HD2	1.77	0.41
1:A:331:ARG:NH1	1:A:331:ARG:CG	2.58	0.41
1:A:347:LEU:HD22	1:A:347:LEU:O	2.20	0.41
1:A:121:MET:SD	1:A:152:PRO:HG2	2.60	0.41
1:B:378:ILE:O	1:B:382:LYS:HG2	2.20	0.41
1:A:121:MET:CG	1:A:152:PRO:HG2	2.50	0.41
1:A:217:ARG:HD3	1:A:250:PHE:CE2	2.55	0.41
1:B:313:TRP:O	1:B:317:THR:HB	2.21	0.41
1:C:291:ASN:O	1:C:292:GLN:CB	2.68	0.41
1:A:121:MET:CE	1:A:151:ALA:HB1	2.50	0.41
1:A:169:GLY:HA3	1:A:219:ARG:HE	1.86	0.41
1:A:371:TRP:O	1:A:372:HIS:HB2	2.20	0.41
1:A:371:TRP:HB3	1:A:373:ILE:HG23	2.02	0.41
1:A:288:MET:HE2	1:A:297:ALA:HB2	2.01	0.41
1:C:222:ASN:C	1:C:224:GLY:N	2.79	0.41
1:A:134:LEU:HD21	1:A:184:GLN:HG2	2.03	0.41
1:A:136:ASP:C	1:A:136:ASP:OD1	2.63	0.41
1:A:148:LEU:HD11	1:A:193:PHE:HB2	2.02	0.41
1:A:156:LYS:HE2	1:A:160:GLU:OE2	2.20	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.80	0.41
1:B:140:LEU:HD23	1:B:144:VAL:HG23	2.03	0.41
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.80	0.41
1:C:302:TYR:HB3	1:C:360:HIS:ND1	2.35	0.41
1:C:336:PRO:HG2	1:C:337:ILE:HD12	2.03	0.41
1:C:358:GLU:HG2	1:C:358:GLU:H	1.78	0.41
1:C:346:TYR:HD2	1:C:380:LEU:HD11	1.86	0.41
1:A:114:LEU:HA	1:A:114:LEU:HD23	1.83	0.40
1:A:232:ILE:HD13	1:A:232:ILE:HA	1.74	0.40
1:A:277:LEU:HA	1:A:277:LEU:HD12	1.62	0.40
1:B:195:LEU:CD2	1:B:270:ALA:HA	2.51	0.40
1:B:360:HIS:CD2	1:B:360:HIS:N	2.87	0.40
1:B:333:GLU:O	1:B:335:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:NH1	1:C:355:ARG:CG	2.74	0.40
1:A:263:CYS:N	1:A:264:PRO:CD	2.82	0.40
1:B:302:TYR:HB3	1:B:360:HIS:CE1	2.56	0.40
1:B:333:GLU:O	1:B:335:SER:N	2.54	0.40
1:A:217:ARG:HD3	1:A:250:PHE:CD2	2.56	0.40
1:B:114:LEU:CD1	1:B:129:TYR:HE1	2.34	0.40
1:B:173:PHE:CE1	1:C:231:ASP:CB	3.05	0.40
1:B:316:LEU:CD1	1:B:357:LEU:HD11	2.51	0.40
1:C:211:LEU:O	1:C:215:THR:HG23	2.21	0.40
1:A:259:ILE:O	1:A:264:PRO:HG3	2.22	0.40
1:B:113:GLU:O	1:B:117:LEU:HG	2.22	0.40
1:C:144:VAL:HG12	1:C:148:LEU:CD1	2.52	0.40
1:C:219:ARG:O	1:C:223:GLU:HG3	2.21	0.40
1:C:230:SER:O	1:C:231:ASP:C	2.65	0.40
1:C:330:THR:O	1:C:330:THR:OG1	2.32	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	284/289 (98%)	255 (90%)	28 (10%)	1 (0%)	30	59
1	B	283/289 (98%)	255 (90%)	25 (9%)	3 (1%)	11	38
1	C	282/289 (98%)	243 (86%)	39 (14%)	0	100	100
All	All	849/867 (98%)	753 (89%)	92 (11%)	4 (0%)	24	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	B	177	THR

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Mol	Chain	Res	Type
1	B	392	GLU
1	B	175	LYS

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	249/251 (99%)	202 (81%)	47 (19%)	1	6
1	B	248/251 (99%)	195 (79%)	53 (21%)	1	4
1	C	247/251 (98%)	191 (77%)	56 (23%)	1	4
All	All	744/753 (99%)	588 (79%)	156 (21%)	1	5

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	A	121	MET
1	A	122	ARG
1	A	123	SER
1	A	132	SER
1	A	140	LEU
1	A	148	LEU
1	A	159	LEU
1	A	162	ILE
1	A	167	LEU
1	A	168	GLN
1	A	179	MET
1	A	189	ILE
1	A	190	LEU
1	A	199	THR
1	A	200	GLU
1	A	206	LYS
1	A	220	LEU
1	A	222	ASN
1	A	227	SER

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Mol	Chain	Res	Type
1	A	231	ASP
1	A	235	ARG
1	A	237	LEU
1	A	244	PHE
1	A	267	ILE
1	A	275	ARG
1	A	277	LEU
1	A	281	VAL
1	A	283	ASP
1	A	285	ILE
1	A	293	MET
1	A	294	ASN
1	A	303	THR
1	A	306	LEU
1	A	317	THR
1	A	327	TRP
1	A	330	THR
1	A	331	ARG
1	A	339	LEU
1	A	343	ASN
1	A	347	LEU
1	A	348	SER
1	A	352	SER
1	A	354	THR
1	A	367	LEU
1	A	376	LYS
1	A	384	MET
1	B	114	LEU
1	B	123	SER
1	B	139	LYS
1	B	140	LEU
1	B	148	LEU
1	B	157	LEU
1	B	161	CYS
1	B	162	ILE
1	B	166	PHE
1	B	167	LEU
1	B	177	THR
1	B	180	VAL
1	B	189	ILE
1	B	198	CYS
1	B	199	THR

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Mol	Chain	Res	Type
1	B	201	MET
1	B	202	GLU
1	B	205	VAL
1	B	215	THR
1	B	226	VAL
1	B	227	SER
1	B	230	SER
1	B	231	ASP
1	B	232	ILE
1	B	237	LEU
1	B	238	LEU
1	B	240	LEU
1	B	265	LYS
1	B	269	ASP
1	B	275	ARG
1	B	277	LEU
1	B	281	VAL
1	B	285	ILE
1	B	292	GLN
1	B	293	MET
1	B	303	THR
1	B	307	GLU
1	B	314	LYS
1	B	317	THR
1	B	330	THR
1	B	333	GLU
1	B	335	SER
1	B	339	LEU
1	B	343	ASN
1	B	350	MET
1	B	351	LYS
1	B	352	SER
1	B	362	VAL
1	B	367	LEU
1	B	372	HIS
1	B	373	ILE
1	B	384	MET
1	B	389	LYS
1	C	111	VAL
1	C	114	LEU
1	C	117	LEU
1	C	123	SER

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Mol	Chain	Res	Type
1	C	137	VAL
1	C	141	ARG
1	C	143	GLU
1	C	148	LEU
1	C	153	LYS
1	C	157	LEU
1	C	159	LEU
1	C	162	ILE
1	C	165	PHE
1	C	166	PHE
1	C	170	SER
1	C	171	LYS
1	C	179	MET
1	C	180	VAL
1	C	184	GLN
1	C	186	SER
1	C	198	CYS
1	C	199	THR
1	C	201	MET
1	C	202	GLU
1	C	211	LEU
1	C	220	LEU
1	C	227	SER
1	C	230	SER
1	C	231	ASP
1	C	235	ARG
1	C	237	LEU
1	C	238	LEU
1	C	239	LEU
1	C	240	LEU
1	C	241	VAL
1	C	259	ILE
1	C	267	ILE
1	C	269	ASP
1	C	273	ARG
1	C	280	ARG
1	C	281	VAL
1	C	284	VAL
1	C	288	MET
1	C	295	VAL
1	C	303	THR
1	C	306	LEU

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Mol	Chain	Res	Type
1	C	324	LYS
1	C	331	ARG
1	C	339	LEU
1	C	350	MET
1	C	351	LYS
1	C	355	ARG
1	C	367	LEU
1	C	378	ILE
1	C	382	LYS
1	C	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	343	ASN
1	B	294	ASN
1	B	345	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	286/289 (98%)	0.26	12 (4%) 40 26	79, 119, 181, 257	0
1	B	285/289 (98%)	0.23	19 (6%) 24 16	69, 106, 173, 234	0
1	C	284/289 (98%)	0.34	11 (3%) 43 29	73, 120, 185, 297	0
All	All	855/867 (98%)	0.28	42 (4%) 35 23	69, 114, 184, 297	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	163	GLY	8.1
1	A	107	ALA	5.6
1	B	170	SER	4.8
1	A	177	THR	4.7
1	C	153	LYS	4.5
1	C	165	PHE	4.0
1	A	168	GLN	3.6
1	B	163	GLY	3.6
1	A	165	PHE	3.5
1	C	172	ALA	3.3
1	B	308	GLU	3.3
1	B	110	SER	3.2
1	C	177	THR	3.2
1	A	391	MET	3.1
1	B	168	GLN	3.1
1	B	390	LYS	3.0
1	B	330	THR	2.9
1	B	379	GLN	2.8
1	B	329	ARG	2.6
1	C	386	ASP	2.6
1	B	369	SER	2.6
1	B	177	THR	2.6
1	C	112	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	175	LYS	2.4
1	B	326	GLU	2.4
1	B	182	SER	2.4
1	C	164	ARG	2.3
1	C	170	SER	2.3
1	C	116	PHE	2.3
1	A	332	GLU	2.2
1	B	175	LYS	2.2
1	A	180	VAL	2.2
1	B	328	LYS	2.2
1	A	338	ARG	2.1
1	A	266	GLU	2.1
1	B	169	GLY	2.1
1	B	292	GLN	2.1
1	A	108	GLN	2.1
1	B	253	GLU	2.0
1	A	335	SER	2.0
1	C	379	GLN	2.0
1	B	111	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.