



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:00 AM UTC

PDB ID : 1E57 / pdb_00001e57
Title : PHYSALIS MOTTLE VIRUS: EMPTY CAPSID
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Deposited on : 2000-07-18
Resolution : 3.20 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

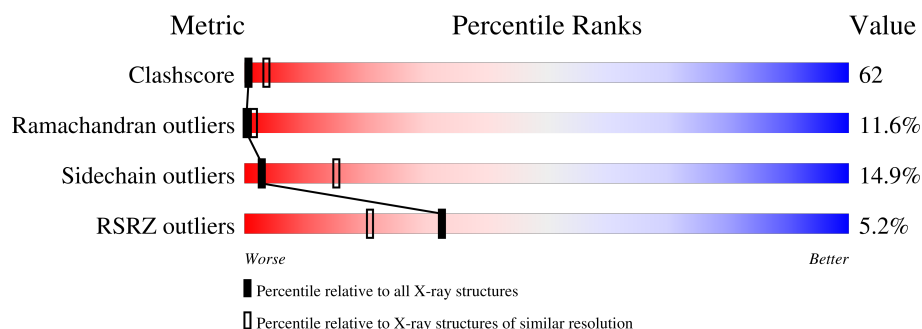
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	188	3% 25% 40% 18% • 15%
1	B	188	7% 30% 47% 19% • •
1	C	188	5% 30% 47% 17% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3742 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.

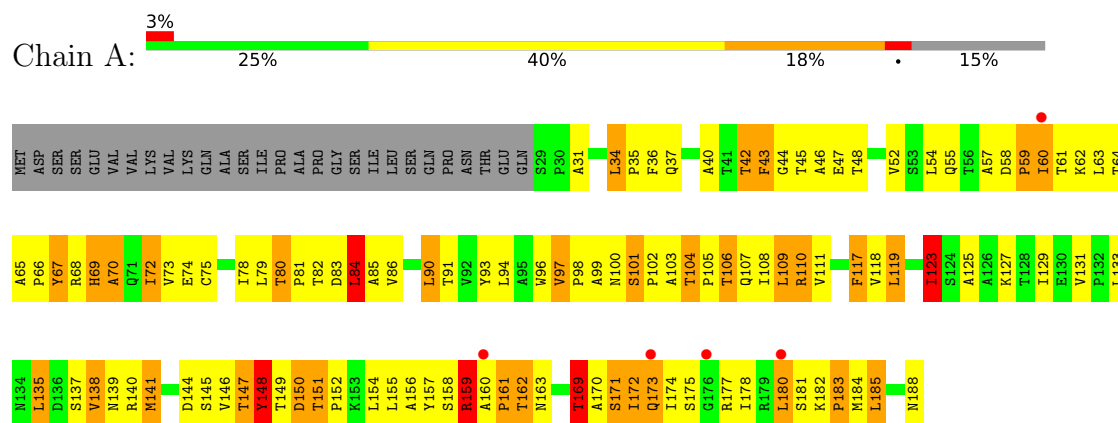
- Molecule 1 is a protein called PHYSALIS MOTTLE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1127	721	183	220	3			
1	B	183	Total	C	N	O	S	0	0	0
			1314	837	218	256	3			
1	C	179	Total	C	N	O	S	0	0	0
			1301	826	217	255	3			

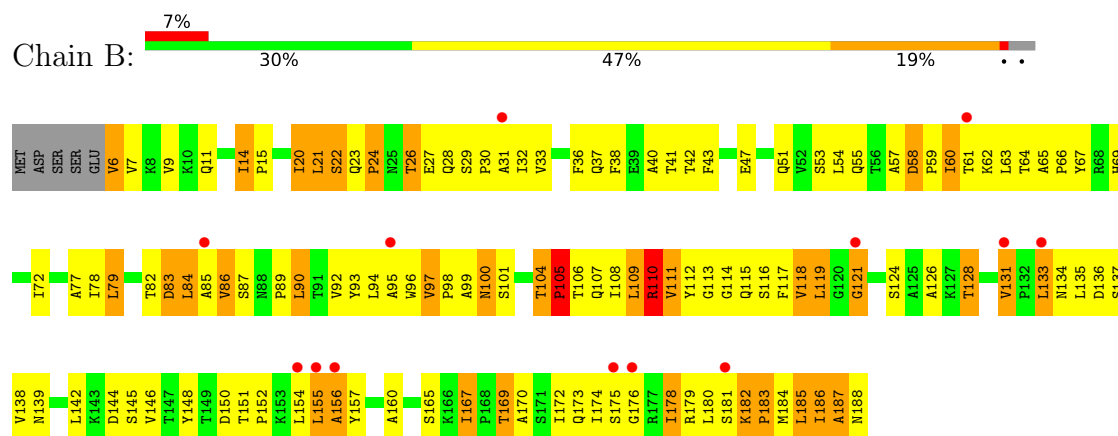
3 Residue-property plots

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.

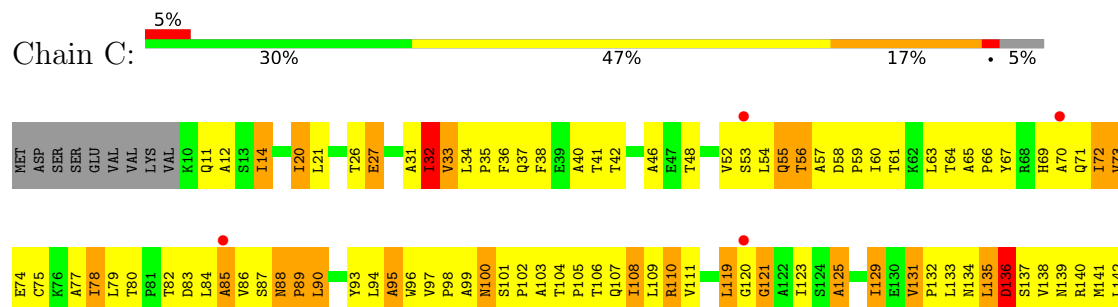
• Molecule 1: PHYSALIS MOTTLE VIRUS



• Molecule 1: PHYSALIS MOTTLE VIRUS



• Molecule 1: PHYSALIS MOTTLE VIRUS



K143	D144	T149	D150	T151	P152	K153	L154	L155	A156	Y157	S158	R159	A160	P161	K166	I167	P168	T169	A170	S171	I172	Q173	I174	S175	G176	R177	I178	R179	L180	S181	K182	F183	M184	L185	I186	A187	N188
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	289.64Å 287.72Å 295.23Å 63.59° 61.39° 62.94°	Depositor
Resolution (Å)	10.00 – 3.20 10.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	22.6 (10.00-3.20) 33.7 (10.00-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.21Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.279 , 0.296 0.509 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.027 for l,h,k 0.027 for k,l,h 0.035 for -k,-h,-l 0.034 for -h,-l,-k 0.029 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.08	EDS
Total number of atoms	3742	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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	0.77	0/1152	1.17	14/1594 (0.9%)
1	B	0.76	0/1342	1.15	10/1851 (0.5%)
1	C	0.77	0/1330	1.23	18/1834 (1.0%)
All	All	0.76	0/3824	1.19	42/5279 (0.8%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	VAL	N-CA-C	10.78	126.80	108.90
1	C	136	ASP	N-CA-C	-8.54	101.85	113.30
1	C	125	ALA	N-CA-C	-7.24	104.48	113.38
1	A	181	SER	N-CA-C	7.22	117.51	108.19
1	A	131	VAL	CA-C-N	7.20	127.77	120.14
1	A	131	VAL	C-N-CA	7.20	127.77	120.14
1	C	170	ALA	N-CA-C	7.03	119.07	108.46
1	C	129	ILE	N-CA-C	7.02	117.76	107.37
1	B	131	VAL	CA-C-N	7.01	127.26	119.90
1	B	131	VAL	C-N-CA	7.01	127.26	119.90
1	B	101	SER	CA-C-N	6.81	126.95	119.87
1	B	101	SER	C-N-CA	6.81	126.95	119.87
1	C	32	ILE	N-CA-C	6.68	120.08	113.53
1	B	86	VAL	N-CA-C	-6.67	104.32	113.00
1	C	169	THR	N-CA-C	-6.66	105.06	113.72
1	B	182	LYS	CA-C-N	6.60	128.09	119.84
1	B	182	LYS	C-N-CA	6.60	128.09	119.84
1	A	150	ASP	N-CA-C	-6.27	103.77	112.30
1	B	169	THR	N-CA-C	-6.19	106.32	114.31
1	A	170	ALA	N-CA-C	6.18	118.53	108.76
1	A	43	PHE	N-CA-C	-6.08	100.50	109.62
1	C	56	THR	N-CA-C	6.06	118.18	110.61
1	C	32	ILE	CB-CA-C	-6.05	104.72	110.65
1	C	166	LYS	N-CA-C	-6.03	106.56	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	THR	N-CA-C	5.93	118.13	108.63
1	A	70	ALA	N-CA-C	5.93	118.34	108.13
1	C	131	VAL	CA-C-N	5.78	127.06	119.84
1	C	131	VAL	C-N-CA	5.78	127.06	119.84
1	A	119	LEU	N-CA-C	5.66	117.88	108.99
1	A	169	THR	N-CA-C	-5.58	107.01	113.88
1	A	127	LYS	N-CA-C	5.53	119.47	111.56
1	C	110	ARG	N-CA-C	-5.41	106.26	112.92
1	A	80	THR	N-CA-C	5.32	118.82	107.91
1	C	88	ASN	CA-C-N	5.29	126.45	119.84
1	C	88	ASN	C-N-CA	5.29	126.45	119.84
1	A	110	ARG	N-CA-C	-5.20	107.00	113.19
1	B	170	ALA	N-CA-C	5.19	116.30	108.46
1	A	171	SER	N-CA-C	5.17	119.06	111.04
1	C	186	ILE	N-CA-C	5.13	120.01	109.34
1	C	178	ILE	N-CA-C	5.09	115.69	108.42
1	C	38	PHE	N-CA-C	5.08	116.79	109.07
1	C	137	SER	N-CA-C	-5.01	107.34	113.50

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	1127	0	1095	130	0
1	B	1314	0	1303	180	0
1	C	1301	0	1290	159	0
All	All	3742	0	3688	458	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 62.

All (458) 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:C:154:LEU:HD22	1:C:155:LEU:H	1.15	1.09
1:C:41:THR:H	1:C:172:ILE:HD11	0.96	1.04
1:C:72:ILE:HD13	1:C:73:VAL:N	1.73	1.03
1:B:118:VAL:HG23	1:B:119:LEU:H	1.24	1.02
1:B:11:GLN:NE2	1:B:96:TRP:H	1.61	0.98
1:C:41:THR:H	1:C:172:ILE:CD1	1.76	0.97
1:C:34:LEU:HD12	1:C:35:PRO:HD2	1.42	0.97
1:C:139:ASN:HB2	1:C:150:ASP:HB2	1.45	0.95
1:B:11:GLN:HE22	1:B:96:TRP:N	1.63	0.95
1:A:146:VAL:HG12	1:A:147:THR:H	1.28	0.95
1:A:159:ARG:HG2	1:A:161:PRO:HD3	1.49	0.94
1:C:41:THR:N	1:C:172:ILE:HD11	1.80	0.94
1:C:154:LEU:HD22	1:C:155:LEU:N	1.81	0.93
1:B:138:VAL:HG21	1:B:152:PRO:HG3	1.50	0.92
1:B:84:LEU:HD11	1:B:169:THR:HA	1.52	0.91
1:C:72:ILE:HG22	1:C:140:ARG:O	1.74	0.88
1:B:57:ALA:HB3	1:B:60:ILE:HB	1.54	0.87
1:B:98:PRO:HG3	1:B:138:VAL:HG12	1.54	0.87
1:C:40:ALA:HB3	1:C:172:ILE:HD13	1.56	0.87
1:A:138:VAL:HG21	1:A:152:PRO:HG3	1.56	0.84
1:C:96:TRP:CZ3	1:C:154:LEU:HB2	2.12	0.84
1:B:154:LEU:HD12	1:B:155:LEU:H	1.44	0.81
1:C:79:LEU:HB3	1:C:129:ILE:HB	1.61	0.81
1:A:158:SER:O	1:A:159:ARG:HB3	1.79	0.81
1:B:107:GLN:C	1:B:109:LEU:H	1.88	0.81
1:C:72:ILE:HA	1:C:178:ILE:HG22	1.61	0.80
1:A:108:ILE:O	1:A:109:LEU:HB3	1.78	0.80
1:C:155:LEU:HD12	1:C:155:LEU:O	1.82	0.80
1:A:154:LEU:HD12	1:A:155:LEU:H	1.47	0.80
1:A:148:TYR:HD1	1:A:148:TYR:H	1.28	0.79
1:C:139:ASN:HB2	1:C:150:ASP:CB	2.12	0.79
1:B:20:ILE:O	1:C:21:LEU:HB3	1.82	0.79
1:A:84:LEU:HD23	1:A:84:LEU:H	1.47	0.79
1:C:41:THR:HG22	1:C:172:ILE:HG12	1.64	0.78
1:B:6:VAL:N	1:B:128:THR:HG1	1.81	0.78
1:C:178:ILE:HG13	1:C:180:LEU:HD21	1.66	0.78
1:C:54:LEU:O	1:C:60:ILE:HD11	1.83	0.78
1:B:154:LEU:HD12	1:B:155:LEU:N	1.98	0.78
1:C:58:ASP:HB2	1:C:59:PRO:HD3	1.65	0.77
1:C:179:ARG:O	1:C:180:LEU:HD23	1.82	0.77
1:B:31:ALA:HB2	1:B:181:SER:HB3	1.67	0.77
1:B:107:GLN:O	1:B:109:LEU:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HA	1:C:125:ALA:HB1	1.66	0.76
1:B:72:ILE:HG23	1:B:142:LEU:HD23	1.68	0.76
1:A:72:ILE:HD12	1:A:73:VAL:H	1.48	0.76
1:A:45:THR:HG23	1:A:46:ALA:H	1.47	0.76
1:C:179:ARG:C	1:C:180:LEU:HD23	2.09	0.76
1:B:40:ALA:HB3	1:B:172:ILE:HB	1.68	0.75
1:A:109:LEU:HD23	1:A:109:LEU:C	2.12	0.75
1:C:32:ILE:HD13	1:C:32:ILE:H	1.51	0.75
1:C:135:LEU:HD12	1:C:140:ARG:HG2	1.67	0.74
1:B:11:GLN:HE22	1:B:96:TRP:H	0.82	0.74
1:A:185:LEU:HD22	1:A:185:LEU:H	1.50	0.74
1:A:78:ILE:HD11	1:A:173:GLN:CB	2.16	0.74
1:B:47:GLU:HB2	1:B:160:ALA:HB2	1.69	0.74
1:C:184:MET:HA	1:C:184:MET:HE3	1.70	0.73
1:C:178:ILE:CG1	1:C:180:LEU:HD21	2.19	0.73
1:A:93:TYR:O	1:A:156:ALA:HA	1.89	0.73
1:A:144:ASP:CG	1:A:145:SER:H	1.97	0.73
1:A:66:PRO:HB2	1:A:67:TYR:CE1	2.26	0.71
1:C:73:VAL:HG23	1:C:178:ILE:HA	1.72	0.70
1:A:154:LEU:HD12	1:A:155:LEU:N	2.05	0.70
1:B:174:ILE:HG13	1:B:174:ILE:O	1.91	0.70
1:C:70:ALA:HB3	1:C:143:LYS:HB3	1.72	0.70
1:C:41:THR:CG2	1:C:172:ILE:HG12	2.22	0.70
1:B:135:LEU:HD23	1:B:135:LEU:H	1.57	0.69
1:B:54:LEU:HD12	1:B:152:PRO:HB2	1.74	0.69
1:B:97:VAL:HG23	1:B:98:PRO:HD2	1.73	0.69
1:B:72:ILE:HD12	1:B:72:ILE:C	2.18	0.69
1:B:14:ILE:HG12	1:B:15:PRO:HD2	1.74	0.69
1:B:57:ALA:O	1:B:58:ASP:C	2.35	0.69
1:C:119:LEU:N	1:C:119:LEU:HD23	2.07	0.69
1:A:148:TYR:HA	1:B:146:VAL:HG12	1.75	0.68
1:B:21:LEU:HD22	1:B:22:SER:H	1.58	0.68
1:C:178:ILE:CD1	1:C:180:LEU:HD21	2.23	0.68
1:A:79:LEU:HB3	1:A:129:ILE:HG13	1.76	0.68
1:B:31:ALA:CB	1:B:181:SER:HB3	2.24	0.68
1:B:96:TRP:CE2	1:B:133:LEU:HB2	2.29	0.68
1:C:176:GLY:C	1:C:177:ARG:HG3	2.17	0.68
1:C:32:ILE:H	1:C:32:ILE:CD1	2.08	0.67
1:A:146:VAL:HG12	1:A:147:THR:N	2.07	0.67
1:A:72:ILE:HD12	1:A:73:VAL:N	2.09	0.67
1:A:123:ILE:O	1:A:123:ILE:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD23	1:C:135:LEU:H	1.59	0.66
1:B:100:ASN:C	1:B:100:ASN:HD22	2.03	0.66
1:C:82:THR:C	1:C:84:LEU:H	2.04	0.66
1:A:117:PHE:CD1	1:A:117:PHE:N	2.65	0.65
1:B:28:GLN:HG3	1:B:29:SER:H	1.61	0.65
1:A:106:THR:C	1:A:108:ILE:H	2.04	0.65
1:B:118:VAL:O	1:B:119:LEU:HB2	1.95	0.65
1:A:172:ILE:HG22	1:A:172:ILE:O	1.98	0.64
1:A:155:LEU:N	1:A:155:LEU:HD12	2.11	0.64
1:B:118:VAL:HG23	1:B:119:LEU:N	2.03	0.64
1:C:134:ASN:C	1:C:136:ASP:H	2.04	0.64
1:B:66:PRO:HG2	1:B:67:TYR:CE2	2.33	0.64
1:A:110:ARG:HG2	1:B:188:ASN:HB3	1.78	0.64
1:B:98:PRO:C	1:B:100:ASN:H	2.06	0.64
1:C:101:SER:C	1:C:103:ALA:H	2.05	0.64
1:C:139:ASN:OD1	1:C:141:MET:HB2	1.97	0.64
1:A:58:ASP:HB3	1:A:59:PRO:HD3	1.79	0.64
1:C:142:LEU:O	1:C:142:LEU:HD23	1.98	0.64
1:C:82:THR:O	1:C:84:LEU:N	2.30	0.64
1:C:133:LEU:HD23	1:C:133:LEU:H	1.63	0.63
1:C:171:SER:OG	1:C:172:ILE:N	2.30	0.63
1:A:37:GLN:HA	1:A:174:ILE:O	1.98	0.63
1:A:66:PRO:HB2	1:A:67:TYR:CD1	2.33	0.63
1:C:55:GLN:HA	1:C:142:LEU:HD21	1.81	0.63
1:C:57:ALA:O	1:C:58:ASP:C	2.41	0.63
1:A:84:LEU:O	1:A:86:VAL:N	2.31	0.62
1:B:77:ALA:HB3	1:B:131:VAL:O	1.99	0.62
1:A:140:ARG:O	1:A:141:MET:C	2.42	0.62
1:B:14:ILE:HD13	1:B:15:PRO:N	2.15	0.62
1:B:43:PHE:CE2	1:B:92:VAL:HG12	2.34	0.62
1:C:119:LEU:N	1:C:119:LEU:CD2	2.63	0.62
1:B:94:LEU:HA	1:B:156:ALA:HB2	1.82	0.62
1:A:81:PRO:HG3	1:A:119:LEU:HD23	1.82	0.62
1:A:79:LEU:HB3	1:A:129:ILE:CG1	2.29	0.61
1:B:32:ILE:HD12	1:B:33:VAL:H	1.64	0.61
1:B:61:THR:C	1:B:63:LEU:N	2.58	0.61
1:C:107:GLN:O	1:C:109:LEU:N	2.33	0.61
1:A:111:VAL:HG13	1:B:186:ILE:O	2.01	0.61
1:B:134:ASN:C	1:B:134:ASN:HD22	2.08	0.61
1:B:60:ILE:O	1:B:64:THR:HG23	1.99	0.61
1:C:167:ILE:HB	1:C:168:PRO:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD12	1:A:180:LEU:O	2.01	0.61
1:C:20:ILE:HD13	1:C:20:ILE:H	1.65	0.61
1:C:54:LEU:O	1:C:56:THR:N	2.34	0.61
1:A:67:TYR:CD1	1:A:67:TYR:N	2.69	0.61
1:B:21:LEU:HA	1:C:21:LEU:HD22	1.83	0.60
1:B:146:VAL:HG23	1:B:146:VAL:O	2.00	0.60
1:C:93:TYR:O	1:C:94:LEU:HB2	1.99	0.60
1:C:178:ILE:HD12	1:C:180:LEU:HD21	1.83	0.60
1:A:34:LEU:HD23	1:A:35:PRO:CD	2.31	0.60
1:C:61:THR:C	1:C:63:LEU:H	2.10	0.60
1:C:155:LEU:HD12	1:C:155:LEU:C	2.25	0.60
1:A:36:PHE:CD1	1:A:36:PHE:C	2.80	0.60
1:B:172:ILE:O	1:B:172:ILE:HG22	2.01	0.60
1:C:34:LEU:HD12	1:C:35:PRO:CD	2.24	0.60
1:B:78:ILE:HG22	1:B:79:LEU:N	2.16	0.59
1:B:113:GLY:O	1:B:115:GLN:HG3	2.02	0.59
1:B:144:ASP:OD1	1:B:145:SER:N	2.35	0.59
1:B:59:PRO:HG2	1:B:60:ILE:H	1.68	0.59
1:B:172:ILE:O	1:B:174:ILE:HG23	2.03	0.59
1:B:55:GLN:HB2	1:B:151:THR:HG21	1.84	0.59
1:B:37:GLN:HG3	1:B:175:SER:HB3	1.85	0.58
1:C:120:GLY:H	1:C:125:ALA:CB	2.17	0.58
1:A:144:ASP:OD1	1:A:145:SER:N	2.36	0.58
1:B:28:GLN:HG3	1:B:29:SER:N	2.19	0.58
1:A:96:TRP:CZ3	1:A:154:LEU:HB2	2.39	0.58
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.68	0.58
1:A:31:ALA:HB1	1:A:180:LEU:H	1.68	0.58
1:A:90:LEU:HD21	1:A:169:THR:HG21	1.85	0.58
1:A:135:LEU:N	1:A:135:LEU:HD12	2.19	0.58
1:C:61:THR:C	1:C:63:LEU:N	2.59	0.58
1:B:90:LEU:N	1:B:90:LEU:CD2	2.67	0.58
1:B:90:LEU:N	1:B:90:LEU:HD23	2.18	0.58
1:A:80:THR:HB	1:A:171:SER:HB3	1.85	0.58
1:C:134:ASN:O	1:C:136:ASP:N	2.37	0.57
1:B:84:LEU:HD12	1:B:85:ALA:N	2.18	0.57
1:B:135:LEU:H	1:B:135:LEU:CD2	2.17	0.57
1:C:82:THR:C	1:C:84:LEU:N	2.60	0.57
1:C:181:SER:O	1:C:182:LYS:C	2.47	0.57
1:A:78:ILE:O	1:A:172:ILE:HA	2.04	0.57
1:C:149:THR:C	1:C:151:THR:H	2.12	0.57
1:B:184:MET:HG3	1:B:185:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ILE:CD1	1:C:32:ILE:N	2.67	0.57
1:A:61:THR:C	1:A:63:LEU:H	2.13	0.56
1:B:61:THR:C	1:B:63:LEU:H	2.13	0.56
1:C:84:LEU:O	1:C:86:VAL:N	2.38	0.56
1:B:135:LEU:HD23	1:B:135:LEU:N	2.21	0.56
1:B:87:SER:C	1:B:89:PRO:HD3	2.31	0.56
1:C:75:CYS:HB3	1:C:133:LEU:HD21	1.88	0.56
1:C:33:VAL:HG12	1:C:33:VAL:O	2.05	0.56
1:C:74:GLU:HB3	1:C:177:ARG:HD3	1.88	0.56
1:B:98:PRO:C	1:B:100:ASN:N	2.63	0.56
1:B:104:THR:HG23	1:B:107:GLN:CG	2.35	0.56
1:C:72:ILE:HD13	1:C:72:ILE:C	2.31	0.56
1:A:58:ASP:O	1:A:59:PRO:C	2.49	0.56
1:C:186:ILE:HD12	1:C:186:ILE:C	2.31	0.56
1:B:178:ILE:HG12	1:B:179:ARG:H	1.70	0.55
1:B:98:PRO:O	1:B:100:ASN:N	2.39	0.55
1:B:96:TRP:CZ3	1:B:154:LEU:HB2	2.42	0.55
1:C:37:GLN:HA	1:C:174:ILE:O	2.07	0.55
1:C:119:LEU:HD23	1:C:119:LEU:H	1.70	0.55
1:B:72:ILE:HG23	1:B:142:LEU:CD2	2.37	0.55
1:B:184:MET:HG3	1:B:185:LEU:N	2.22	0.55
1:B:186:ILE:HG13	1:B:187:ALA:N	2.22	0.55
1:C:84:LEU:CB	1:C:169:THR:HG23	2.37	0.55
1:A:70:ALA:HB2	1:A:180:LEU:HB3	1.87	0.55
1:B:100:ASN:C	1:B:100:ASN:ND2	2.64	0.55
1:C:71:GLN:O	1:C:178:ILE:HB	2.07	0.55
1:B:116:SER:C	1:B:117:PHE:CD1	2.85	0.55
1:C:14:ILE:O	1:C:14:ILE:HD12	2.07	0.55
1:A:52:VAL:CG2	1:A:154:LEU:HB3	2.37	0.54
1:B:31:ALA:HB2	1:B:181:SER:CB	2.35	0.54
1:B:78:ILE:HB	1:B:173:GLN:O	2.07	0.54
1:B:111:VAL:HG23	1:B:112:TYR:H	1.73	0.54
1:C:60:ILE:O	1:C:64:THR:HG23	2.08	0.54
1:C:171:SER:O	1:C:172:ILE:HG23	2.07	0.54
1:A:54:LEU:N	1:A:54:LEU:HD22	2.23	0.54
1:A:101:SER:C	1:A:103:ALA:H	2.15	0.54
1:B:138:VAL:CG2	1:B:152:PRO:HG3	2.33	0.54
1:A:43:PHE:HA	1:A:48:THR:CB	2.38	0.54
1:C:65:ALA:N	1:C:66:PRO:HD2	2.23	0.54
1:B:135:LEU:C	1:B:137:SER:N	2.65	0.53
1:A:91:THR:HG22	1:A:118:VAL:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:HB3	1:A:149:THR:O	2.09	0.53
1:B:24:PRO:HG3	1:B:28:GLN:HG2	1.91	0.53
1:B:61:THR:O	1:B:63:LEU:N	2.42	0.53
1:B:178:ILE:HD13	1:B:179:ARG:N	2.24	0.53
1:C:94:LEU:O	1:C:95:ALA:HB2	2.07	0.53
1:A:150:ASP:OD1	1:B:145:SER:HA	2.09	0.53
1:C:135:LEU:HD23	1:C:135:LEU:N	2.23	0.53
1:C:141:MET:HE2	1:C:144:ASP:OD2	2.09	0.53
1:B:85:ALA:C	1:B:87:SER:N	2.67	0.53
1:B:96:TRP:CD1	1:B:133:LEU:HA	2.44	0.53
1:B:53:SER:C	1:B:55:GLN:N	2.65	0.52
1:C:78:ILE:O	1:C:172:ILE:HA	2.08	0.52
1:C:98:PRO:C	1:C:100:ASN:H	2.17	0.52
1:A:82:THR:O	1:A:83:ASP:C	2.52	0.52
1:C:20:ILE:HG22	1:C:139:ASN:HD21	1.74	0.52
1:B:97:VAL:HG23	1:B:98:PRO:CD	2.37	0.52
1:C:90:LEU:N	1:C:90:LEU:CD2	2.72	0.52
1:C:96:TRP:CG	1:C:133:LEU:HB3	2.44	0.52
1:A:109:LEU:HD23	1:A:110:ARG:N	2.24	0.52
1:C:100:ASN:OD1	1:C:100:ASN:N	2.42	0.52
1:B:139:ASN:HB2	1:B:150:ASP:HB2	1.91	0.52
1:C:32:ILE:O	1:C:33:VAL:HB	2.09	0.52
1:C:53:SER:HA	1:C:153:LYS:HA	1.91	0.52
1:A:119:LEU:HD12	1:A:119:LEU:N	2.24	0.52
1:B:104:THR:HG23	1:B:107:GLN:CD	2.35	0.52
1:B:84:LEU:CD1	1:B:85:ALA:N	2.73	0.52
1:A:37:GLN:HG3	1:A:175:SER:HB3	1.91	0.51
1:B:21:LEU:HD22	1:B:22:SER:N	2.24	0.51
1:A:70:ALA:CB	1:A:180:LEU:HB3	2.40	0.51
1:A:144:ASP:CG	1:A:145:SER:N	2.67	0.51
1:B:178:ILE:HG12	1:B:179:ARG:N	2.25	0.51
1:B:41:THR:HG22	1:B:42:THR:N	2.26	0.51
1:B:65:ALA:HB3	1:B:66:PRO:HD3	1.91	0.51
1:B:84:LEU:HD12	1:B:84:LEU:C	2.35	0.51
1:C:72:ILE:HD13	1:C:73:VAL:H	1.68	0.51
1:A:90:LEU:O	1:A:119:LEU:HD12	2.11	0.51
1:B:92:VAL:O	1:B:93:TYR:HD1	1.93	0.51
1:C:73:VAL:HG23	1:C:177:ARG:O	2.10	0.51
1:A:34:LEU:HD23	1:A:35:PRO:HD2	1.93	0.51
1:B:83:ASP:O	1:B:84:LEU:O	2.29	0.51
1:B:78:ILE:CG2	1:B:79:LEU:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:C	1:B:137:SER:H	2.19	0.51
1:C:84:LEU:HB3	1:C:169:THR:HG23	1.92	0.51
1:A:158:SER:O	1:A:159:ARG:CB	2.53	0.51
1:B:36:PHE:CE1	1:B:176:GLY:C	2.89	0.51
1:C:96:TRP:CD1	1:C:133:LEU:HB3	2.46	0.51
1:A:185:LEU:H	1:A:185:LEU:CD2	2.22	0.50
1:B:155:LEU:O	1:B:156:ALA:O	2.28	0.50
1:B:178:ILE:CG1	1:B:179:ARG:N	2.73	0.50
1:B:90:LEU:HD23	1:B:90:LEU:H	1.77	0.50
1:C:120:GLY:H	1:C:125:ALA:HB1	1.76	0.50
1:C:134:ASN:C	1:C:136:ASP:N	2.69	0.50
1:C:157:TYR:CD1	1:C:158:SER:N	2.79	0.50
1:A:74:GLU:HG3	1:A:177:ARG:H	1.76	0.50
1:B:85:ALA:C	1:B:87:SER:H	2.18	0.50
1:B:21:LEU:O	1:B:22:SER:O	2.29	0.50
1:A:104:THR:O	1:A:106:THR:N	2.45	0.50
1:A:180:LEU:O	1:A:180:LEU:CD1	2.60	0.50
1:C:66:PRO:HG2	1:C:67:TYR:CD1	2.47	0.50
1:B:14:ILE:HD13	1:B:14:ILE:C	2.37	0.49
1:B:41:THR:CG2	1:B:42:THR:N	2.75	0.49
1:A:54:LEU:HD12	1:A:60:ILE:HD11	1.93	0.49
1:B:63:LEU:N	1:B:63:LEU:HD12	2.27	0.49
1:A:45:THR:HG23	1:A:46:ALA:N	2.23	0.49
1:B:84:LEU:C	1:B:86:VAL:H	2.20	0.49
1:C:52:VAL:O	1:C:52:VAL:HG13	2.13	0.49
1:B:82:THR:O	1:B:83:ASP:C	2.55	0.49
1:C:77:ALA:HB3	1:C:131:VAL:O	2.12	0.49
1:B:93:TYR:C	1:B:156:ALA:HA	2.36	0.49
1:B:134:ASN:C	1:B:134:ASN:ND2	2.69	0.49
1:C:20:ILE:CG2	1:C:139:ASN:HD21	2.26	0.49
1:A:184:MET:O	1:A:185:LEU:C	2.54	0.49
1:C:42:THR:O	1:C:48:THR:HG21	2.13	0.49
1:A:40:ALA:H	1:A:173:GLN:HA	1.78	0.49
1:A:109:LEU:C	1:A:111:VAL:H	2.19	0.49
1:A:118:VAL:O	1:A:119:LEU:HG	2.13	0.49
1:B:11:GLN:NE2	1:B:95:ALA:HA	2.27	0.49
1:C:104:THR:O	1:C:106:THR:N	2.46	0.48
1:B:109:LEU:C	1:B:111:VAL:H	2.21	0.48
1:C:74:GLU:O	1:C:176:GLY:HA2	2.13	0.48
1:A:64:THR:C	1:A:66:PRO:HD2	2.39	0.48
1:A:106:THR:C	1:A:108:ILE:N	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:O	1:B:85:ALA:HB3	2.13	0.48
1:B:172:ILE:O	1:B:173:GLN:C	2.54	0.48
1:A:188:ASN:HD21	1:C:110:ARG:NH2	2.10	0.48
1:C:26:THR:HG22	1:C:27:GLU:CG	2.43	0.48
1:C:84:LEU:O	1:C:85:ALA:C	2.56	0.48
1:C:98:PRO:O	1:C:100:ASN:N	2.47	0.48
1:A:109:LEU:C	1:A:109:LEU:CD2	2.83	0.48
1:C:131:VAL:O	1:C:131:VAL:HG12	2.12	0.48
1:B:178:ILE:HD13	1:B:180:LEU:N	2.29	0.47
1:C:26:THR:HG22	1:C:27:GLU:HG3	1.96	0.47
1:A:46:ALA:C	1:A:160:ALA:HB3	2.40	0.47
1:B:104:THR:HG23	1:B:107:GLN:HG2	1.95	0.47
1:B:117:PHE:CD1	1:B:117:PHE:N	2.82	0.47
1:C:84:LEU:N	1:C:84:LEU:HD22	2.30	0.47
1:C:172:ILE:O	1:C:173:GLN:C	2.56	0.47
1:A:54:LEU:N	1:A:54:LEU:CD2	2.77	0.47
1:A:148:TYR:CD1	1:A:148:TYR:N	2.76	0.47
1:C:72:ILE:HD13	1:C:73:VAL:CA	2.44	0.47
1:C:20:ILE:HD13	1:C:20:ILE:N	2.29	0.47
1:A:138:VAL:HG23	1:A:139:ASN:N	2.29	0.47
1:A:55:GLN:OE1	1:A:151:THR:HG21	2.15	0.47
1:A:109:LEU:C	1:A:111:VAL:N	2.70	0.47
1:B:54:LEU:CD1	1:B:152:PRO:HB2	2.44	0.47
1:C:69:HIS:HD2	1:C:181:SER:OG	1.98	0.46
1:C:72:ILE:HD13	1:C:73:VAL:C	2.40	0.46
1:C:138:VAL:HG21	1:C:152:PRO:HB3	1.97	0.46
1:A:101:SER:O	1:A:103:ALA:N	2.41	0.46
1:C:107:GLN:C	1:C:109:LEU:N	2.72	0.46
1:B:118:VAL:O	1:B:119:LEU:CB	2.63	0.46
1:B:178:ILE:HD13	1:B:178:ILE:C	2.41	0.46
1:A:75:CYS:HB3	1:A:133:LEU:HD23	1.98	0.46
1:C:55:GLN:CB	1:C:151:THR:HG21	2.46	0.46
1:B:89:PRO:HG3	1:B:121:GLY:H	1.81	0.46
1:B:118:VAL:C	1:B:119:LEU:CD1	2.89	0.46
1:B:139:ASN:CB	1:B:150:ASP:HB2	2.46	0.46
1:A:154:LEU:C	1:A:155:LEU:HD12	2.40	0.46
1:A:159:ARG:HG2	1:A:161:PRO:CD	2.34	0.46
1:B:184:MET:CG	1:B:185:LEU:N	2.77	0.46
1:C:85:ALA:O	1:C:86:VAL:C	2.58	0.46
1:C:172:ILE:N	1:C:172:ILE:HD12	2.31	0.46
1:A:60:ILE:HG22	1:A:61:THR:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ILE:HD13	1:C:32:ILE:N	2.19	0.46
1:C:101:SER:HA	1:C:102:PRO:HD3	1.69	0.46
1:B:182:LYS:HA	1:B:183:PRO:HD2	1.71	0.46
1:C:101:SER:C	1:C:103:ALA:N	2.73	0.46
1:B:58:ASP:HB3	1:B:59:PRO:CD	2.46	0.45
1:A:60:ILE:O	1:A:64:THR:HG23	2.17	0.45
1:A:91:THR:HG22	1:A:118:VAL:HG12	1.98	0.45
1:A:182:LYS:O	1:A:183:PRO:O	2.34	0.45
1:A:157:TYR:CD1	1:A:158:SER:N	2.85	0.45
1:B:59:PRO:O	1:B:60:ILE:C	2.60	0.45
1:B:84:LEU:O	1:B:86:VAL:N	2.49	0.45
1:B:105:PRO:HB3	1:B:157:TYR:CB	2.46	0.45
1:A:93:TYR:HB2	1:A:108:ILE:HD13	1.98	0.45
1:B:14:ILE:CG1	1:B:15:PRO:HD2	2.43	0.45
1:C:54:LEU:N	1:C:54:LEU:HD22	2.31	0.45
1:A:98:PRO:HB3	1:A:138:VAL:HG12	1.99	0.45
1:C:61:THR:O	1:C:63:LEU:N	2.50	0.45
1:A:138:VAL:HB	1:A:150:ASP:O	2.17	0.45
1:B:65:ALA:HB3	1:B:66:PRO:CD	2.46	0.45
1:B:119:LEU:N	1:B:119:LEU:HD12	2.31	0.45
1:A:80:THR:HB	1:A:171:SER:CB	2.47	0.45
1:B:43:PHE:HE1	1:B:172:ILE:CG1	2.30	0.45
1:C:135:LEU:H	1:C:135:LEU:CD2	2.29	0.45
1:C:159:ARG:HB2	1:C:159:ARG:CZ	2.46	0.45
1:B:110:ARG:HG2	1:B:110:ARG:NH1	2.30	0.45
1:A:65:ALA:N	1:A:66:PRO:CD	2.80	0.45
1:B:89:PRO:HG3	1:B:121:GLY:N	2.32	0.45
1:B:98:PRO:HG3	1:B:138:VAL:CG1	2.36	0.45
1:B:82:THR:OG1	1:B:84:LEU:HD11	2.17	0.44
1:C:157:TYR:CG	1:C:158:SER:N	2.84	0.44
1:A:34:LEU:HA	1:A:35:PRO:HD3	1.72	0.44
1:A:72:ILE:HA	1:A:178:ILE:HG13	1.98	0.44
1:A:162:THR:HG22	1:A:163:ASN:N	2.32	0.44
1:C:85:ALA:C	1:C:87:SER:N	2.74	0.44
1:B:111:VAL:HG23	1:B:112:TYR:N	2.33	0.44
1:A:96:TRP:CD1	1:A:133:LEU:HA	2.52	0.44
1:C:54:LEU:C	1:C:56:THR:N	2.74	0.44
1:C:54:LEU:HD23	1:C:152:PRO:O	2.18	0.44
1:B:185:LEU:HD12	1:B:185:LEU:HA	1.85	0.44
1:B:23:GLN:CG	1:B:24:PRO:HD2	2.47	0.44
1:B:38:PHE:CD2	1:B:59:PRO:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:C	1:A:63:LEU:N	2.75	0.44
1:B:61:THR:O	1:B:62:LYS:C	2.61	0.44
1:B:165:SER:CB	1:B:167:ILE:HD12	2.48	0.44
1:A:104:THR:C	1:A:106:THR:N	2.75	0.44
1:C:54:LEU:C	1:C:56:THR:H	2.26	0.43
1:B:133:LEU:HD13	1:B:133:LEU:O	2.18	0.43
1:C:26:THR:O	1:C:27:GLU:CB	2.67	0.43
1:A:161:PRO:O	1:A:162:THR:C	2.60	0.43
1:B:185:LEU:O	1:B:186:ILE:HG12	2.17	0.43
1:C:120:GLY:O	1:C:121:GLY:C	2.61	0.43
1:B:38:PHE:CD1	1:B:38:PHE:N	2.87	0.43
1:B:167:ILE:HD12	1:B:167:ILE:H	1.84	0.43
1:A:178:ILE:HG23	1:A:178:ILE:O	2.19	0.43
1:B:22:SER:O	1:B:23:GLN:HB2	2.18	0.43
1:B:65:ALA:N	1:B:66:PRO:HD2	2.34	0.43
1:B:14:ILE:HD13	1:B:15:PRO:CD	2.49	0.43
1:B:62:LYS:C	1:B:63:LEU:HD12	2.42	0.43
1:B:96:TRP:NE1	1:B:133:LEU:HB2	2.34	0.43
1:B:107:GLN:C	1:B:109:LEU:N	2.53	0.43
1:C:32:ILE:HD13	1:C:33:VAL:H	1.82	0.43
1:A:104:THR:O	1:A:107:GLN:N	2.52	0.43
1:C:88:ASN:HA	1:C:89:PRO:HD2	1.88	0.43
1:C:155:LEU:C	1:C:155:LEU:CD1	2.90	0.43
1:A:155:LEU:N	1:A:155:LEU:CD1	2.82	0.43
1:A:148:TYR:HA	1:B:146:VAL:CG1	2.46	0.43
1:B:84:LEU:H	1:B:84:LEU:HG	1.63	0.43
1:C:90:LEU:HD23	1:C:90:LEU:O	2.19	0.43
1:C:20:ILE:HG21	1:C:141:MET:CG	2.49	0.42
1:C:31:ALA:HB3	1:C:179:ARG:HG3	2.01	0.42
1:A:110:ARG:CG	1:B:188:ASN:HB3	2.47	0.42
1:A:118:VAL:C	1:A:119:LEU:HD12	2.43	0.42
1:B:51:GLN:O	1:B:51:GLN:HG3	2.19	0.42
1:C:120:GLY:H	1:C:125:ALA:HB3	1.83	0.42
1:A:34:LEU:O	1:A:177:ARG:HA	2.20	0.42
1:C:111:VAL:O	1:C:111:VAL:HG13	2.20	0.42
1:A:146:VAL:CG1	1:A:147:THR:H	2.10	0.42
1:C:26:THR:O	1:C:27:GLU:HB3	2.19	0.42
1:B:43:PHE:HE1	1:B:172:ILE:HG13	1.84	0.42
1:B:134:ASN:HD21	1:B:136:ASP:HB2	1.83	0.42
1:C:84:LEU:HB2	1:C:169:THR:HG23	2.01	0.42
1:B:26:THR:O	1:B:27:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:PRO:HG2	1:B:67:TYR:CD2	2.55	0.42
1:A:145:SER:CB	1:C:150:ASP:OD2	2.68	0.42
1:B:11:GLN:HE21	1:B:95:ALA:HA	1.83	0.42
1:B:139:ASN:ND2	1:B:148:TYR:CD2	2.88	0.42
1:C:107:GLN:O	1:C:108:ILE:C	2.63	0.42
1:C:58:ASP:HB2	1:C:59:PRO:CD	2.43	0.42
1:C:133:LEU:H	1:C:133:LEU:CD2	2.29	0.42
1:A:68:ARG:O	1:A:69:HIS:HB2	2.20	0.42
1:C:11:GLN:HG2	1:C:12:ALA:O	2.20	0.42
1:C:46:ALA:O	1:C:48:THR:HG23	2.19	0.42
1:A:64:THR:O	1:A:65:ALA:C	2.63	0.41
1:B:178:ILE:CD1	1:B:179:ARG:N	2.83	0.41
1:B:115:GLN:HB2	1:B:117:PHE:HE1	1.85	0.41
1:A:94:LEU:HA	1:A:155:LEU:O	2.21	0.41
1:A:60:ILE:O	1:A:63:LEU:HB3	2.21	0.41
1:B:96:TRP:CG	1:B:133:LEU:HD23	2.56	0.41
1:C:93:TYR:HB3	1:C:108:ILE:CB	2.51	0.41
1:A:68:ARG:O	1:A:69:HIS:CB	2.69	0.41
1:B:9:VAL:O	1:B:9:VAL:HG12	2.18	0.41
1:B:111:VAL:CG2	1:B:112:TYR:H	2.33	0.41
1:B:139:ASN:OD1	1:B:139:ASN:C	2.63	0.41
1:C:149:THR:C	1:C:151:THR:N	2.78	0.41
1:A:97:VAL:HG12	1:B:185:LEU:HD23	2.03	0.41
1:B:53:SER:C	1:B:55:GLN:H	2.29	0.41
1:B:84:LEU:CD2	1:B:167:ILE:HD13	2.51	0.41
1:B:115:GLN:HB2	1:B:117:PHE:CE1	2.56	0.41
1:A:45:THR:CG2	1:A:46:ALA:H	2.26	0.41
1:A:104:THR:C	1:A:106:THR:H	2.29	0.41
1:A:135:LEU:C	1:A:137:SER:H	2.29	0.41
1:B:41:THR:HG22	1:B:42:THR:O	2.20	0.41
1:C:64:THR:C	1:C:66:PRO:HD2	2.45	0.41
1:C:178:ILE:HG13	1:C:180:LEU:CD2	2.44	0.41
1:C:98:PRO:C	1:C:100:ASN:N	2.79	0.41
1:A:123:ILE:O	1:A:123:ILE:CG2	2.67	0.40
1:C:36:PHE:CZ	1:C:176:GLY:HA3	2.56	0.40
1:C:172:ILE:HD12	1:C:172:ILE:C	2.45	0.40
1:A:83:ASP:O	1:A:84:LEU:O	2.38	0.40
1:A:172:ILE:O	1:A:172:ILE:CG2	2.68	0.40
1:C:46:ALA:HA	1:C:161:PRO:HD2	2.02	0.40
1:A:43:PHE:CB	1:A:172:ILE:HD11	2.51	0.40
1:A:80:THR:HA	1:A:81:PRO:HD3	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:O	1:B:114:GLY:C	2.64	0.40
1:C:172:ILE:CD1	1:C:172:ILE:C	2.94	0.40
1:A:78:ILE:HG13	1:A:173:GLN:O	2.21	0.40
1:B:29:SER:OG	1:B:30:PRO:HD2	2.21	0.40
1:B:133:LEU:C	1:B:133:LEU:HD22	2.46	0.40
1:C:133:LEU:HD23	1:C:133:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/188 (84%)	91 (58%)	43 (27%)	24 (15%)	0	0
1	B	181/188 (96%)	120 (66%)	40 (22%)	21 (12%)	0	1
1	C	177/188 (94%)	126 (71%)	36 (20%)	15 (8%)	0	3
All	All	516/564 (92%)	337 (65%)	119 (23%)	60 (12%)	0	1

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	84	LEU
1	A	100	ASN
1	A	159	ARG
1	B	22	SER
1	B	26	THR
1	B	84	LEU
1	B	108	ILE
1	B	128	THR
1	B	156	ALA
1	B	183	PRO

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Mol	Chain	Res	Type
1	B	186	ILE
1	B	187	ALA
1	C	27	GLU
1	C	172	ILE
1	A	69	HIS
1	A	125	ALA
1	A	161	PRO
1	A	183	PRO
1	B	24	PRO
1	B	118	VAL
1	B	185	LEU
1	C	55	GLN
1	C	83	ASP
1	C	85	ALA
1	C	99	ALA
1	C	108	ILE
1	C	121	GLY
1	C	135	LEU
1	A	57	ALA
1	A	148	TYR
1	A	172	ILE
1	B	99	ALA
1	B	105	PRO
1	B	124	SER
1	C	123	ILE
1	A	62	LYS
1	A	101	SER
1	A	173	GLN
1	B	110	ARG
1	C	105	PRO
1	A	85	ALA
1	A	102	PRO
1	A	138	VAL
1	A	141	MET
1	A	162	THR
1	B	58	ASP
1	B	126	ALA
1	C	89	PRO
1	C	95	ALA
1	C	173	GLN
1	A	44	GLY
1	A	59	PRO

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Mol	Chain	Res	Type
1	B	119	LEU
1	A	105	PRO
1	A	60	ILE
1	A	123	ILE
1	C	33	VAL
1	B	111	VAL
1	B	121	GLY

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	116/159 (73%)	96 (83%)	20 (17%)	2	10
1	B	140/159 (88%)	120 (86%)	20 (14%)	3	16
1	C	140/159 (88%)	121 (86%)	19 (14%)	3	18
All	All	396/477 (83%)	337 (85%)	59 (15%)	3	15

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	42	THR
1	A	67	TYR
1	A	72	ILE
1	A	84	LEU
1	A	90	LEU
1	A	97	VAL
1	A	104	THR
1	A	106	THR
1	A	109	LEU
1	A	117	PHE
1	A	123	ILE
1	A	135	LEU
1	A	147	THR
1	A	148	TYR

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Mol	Chain	Res	Type
1	A	151	THR
1	A	159	ARG
1	A	169	THR
1	A	180	LEU
1	A	185	LEU
1	B	6	VAL
1	B	14	ILE
1	B	20	ILE
1	B	21	LEU
1	B	60	ILE
1	B	69	HIS
1	B	79	LEU
1	B	83	ASP
1	B	90	LEU
1	B	97	VAL
1	B	100	ASN
1	B	104	THR
1	B	105	PRO
1	B	106	THR
1	B	109	LEU
1	B	110	ARG
1	B	133	LEU
1	B	155	LEU
1	B	167	ILE
1	B	178	ILE
1	C	14	ILE
1	C	20	ILE
1	C	32	ILE
1	C	72	ILE
1	C	73	VAL
1	C	78	ILE
1	C	80	THR
1	C	90	LEU
1	C	97	VAL
1	C	100	ASN
1	C	119	LEU
1	C	132	PRO
1	C	136	ASP
1	C	149	THR
1	C	154	LEU
1	C	171	SER
1	C	172	ILE

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Mol	Chain	Res	Type
1	C	177	ARG
1	C	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	188	ASN
1	B	11	GLN
1	B	28	GLN
1	B	55	GLN
1	B	71	GLN
1	B	100	ASN
1	B	107	GLN
1	B	134	ASN
1	C	23	GLN
1	C	25	ASN
1	C	28	GLN
1	C	69	HIS
1	C	71	GLN
1	C	163	ASN
1	C	188	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	160/188 (85%)	0.09	5 (3%) 51 32	15, 15, 15, 15	0
1	B	183/188 (97%)	0.11	13 (7%) 22 14	15, 15, 15, 15	0
1	C	179/188 (95%)	0.22	9 (5%) 34 22	15, 15, 15, 15	0
All	All	522/564 (92%)	0.14	27 (5%) 33 21	15, 15, 15, 15	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	GLY	9.6
1	A	173	GLN	5.9
1	C	153	LYS	4.7
1	C	120	GLY	4.6
1	B	181	SER	4.3
1	C	156	ALA	4.1
1	A	180	LEU	3.6
1	A	176	GLY	3.5
1	B	61	THR	2.9
1	B	131	VAL	2.9
1	A	60	ILE	2.9
1	B	175	SER	2.8
1	C	53	SER	2.8
1	B	156	ALA	2.7
1	B	31	ALA	2.7
1	A	160	ALA	2.5
1	C	85	ALA	2.5
1	B	85	ALA	2.3
1	B	176	GLY	2.3
1	B	154	LEU	2.3
1	B	155	LEU	2.3
1	C	180	LEU	2.2
1	C	70	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	95	ALA	2.2
1	B	133	LEU	2.1
1	B	121	GLY	2.1
1	C	154	LEU	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.