



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:42 AM UTC

PDB ID : 1W39 / pdb_00001w39
Title : Crystal structure of an artificial top component of turnip yellow mosaic virus
Authors : van Roon, A.M.M.; Bink, H.H.J.; Plaisier, J.R.; Pleij, C.W.A.; Abrahams, J.P.; Pannu, N.S.
Deposited on : 2004-07-14
Resolution : 3.75 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

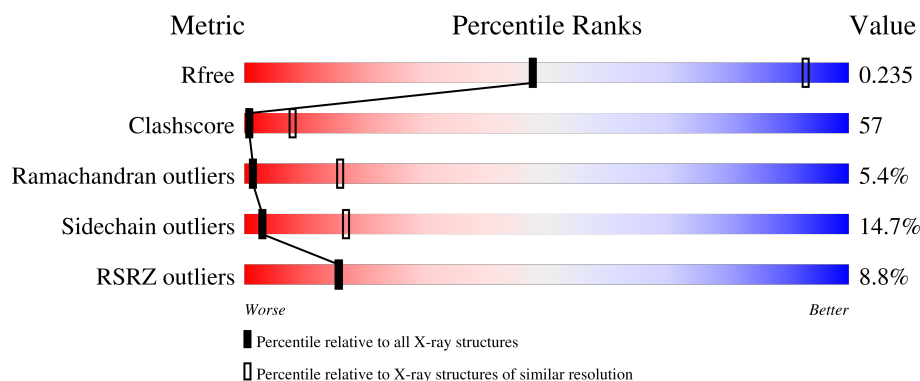
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	189	
1	B	189	
1	C	189	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4094 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.

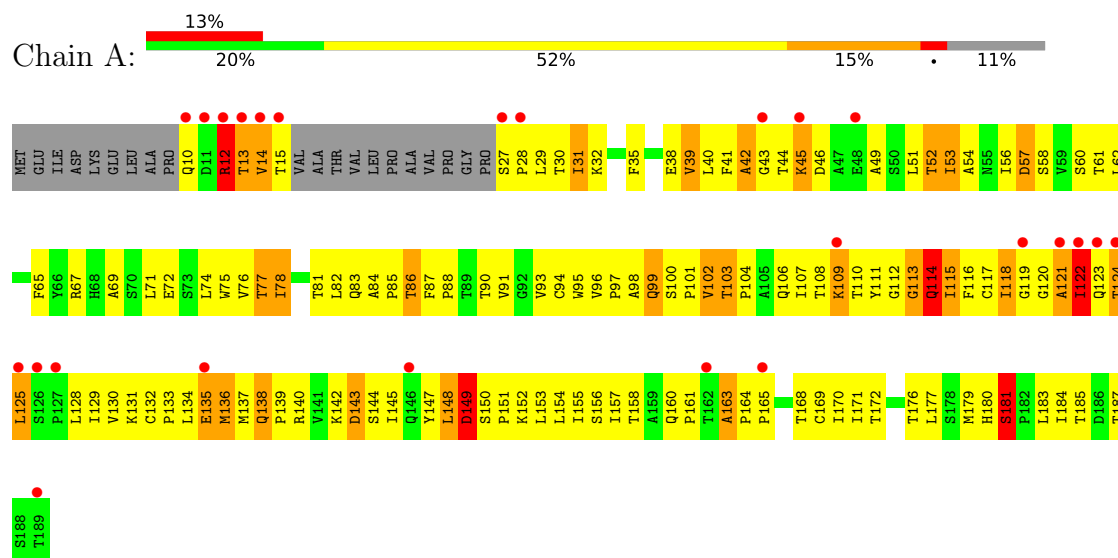
- Molecule 1 is a protein called TURNIP YELLOW MOSAIC VIRUS EMPTY CAPSID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1270	812	204	247	7			
1	B	189	Total	C	N	O	S	0	0	0
			1412	905	225	274	8			
1	C	189	Total	C	N	O	S	0	0	0
			1412	905	225	274	8			

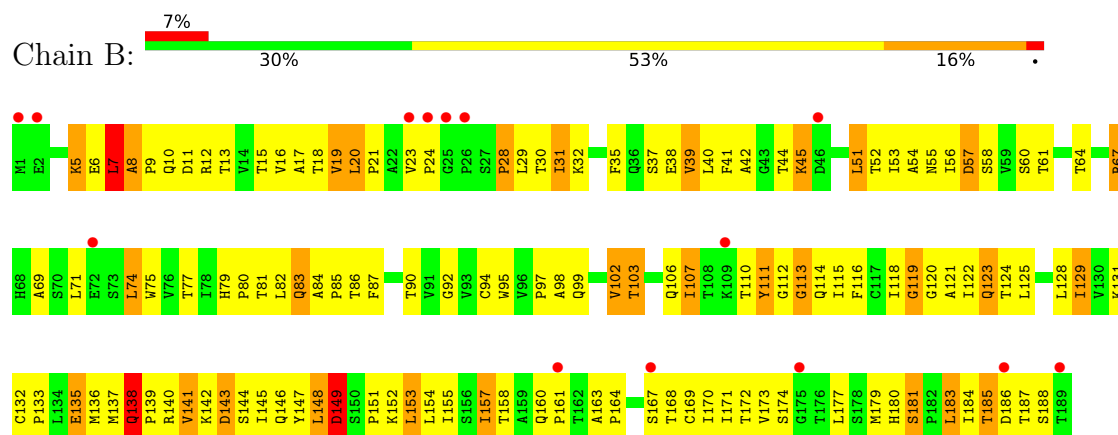
3 Residue-property plots

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.

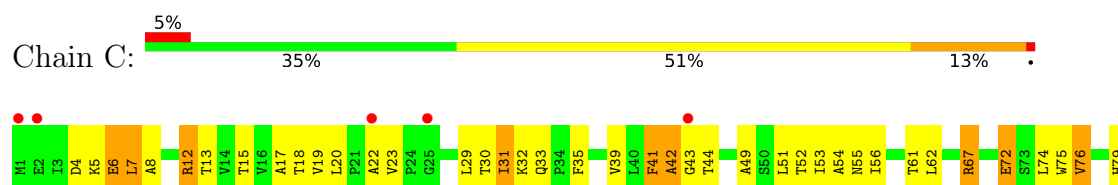
• Molecule 1: TURNIP YELLOW MOSAIC VIRUS EMPTY CAPSID

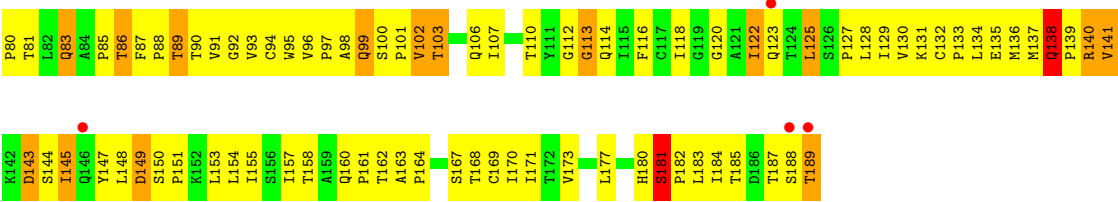


• Molecule 1: TURNIP YELLOW MOSAIC VIRUS EMPTY CAPSID



• Molecule 1: TURNIP YELLOW MOSAIC VIRUS EMPTY CAPSID





4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	688.46 Å 688.46 Å 688.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.75 25.00 – 3.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-3.75) 99.6 (25.00-3.75)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.245 , 0.251 0.230 , 0.235	Depositor DCC
R_{free} test set	7088 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 84.7	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.29	EDS
Total number of atoms	4094	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	0.52	0/1299	0.97	5/1783 (0.3%)
1	B	0.53	0/1446	1.10	13/1989 (0.7%)
1	C	0.56	0/1446	1.11	10/1989 (0.5%)
All	All	0.54	0/4191	1.07	28/5761 (0.5%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ALA	CA-C-N	8.76	129.10	119.90
1	B	8	ALA	C-N-CA	8.76	129.10	119.90
1	C	143	ASP	N-CA-C	7.98	119.08	108.07
1	C	138	GLN	CA-C-N	7.89	129.70	119.84
1	C	138	GLN	C-N-CA	7.89	129.70	119.84
1	C	42	ALA	N-CA-C	7.61	119.62	110.19
1	B	119	GLY	N-CA-C	7.52	119.09	111.95
1	A	42	ALA	N-CA-C	7.06	118.82	108.86
1	C	8	ALA	CA-C-N	7.06	127.45	119.83
1	C	8	ALA	C-N-CA	7.06	127.45	119.83
1	C	181	SER	CA-C-N	6.34	126.29	119.76
1	C	181	SER	C-N-CA	6.34	126.29	119.76
1	B	135	GLU	N-CA-C	-6.33	104.38	111.28
1	B	138	GLN	CA-C-N	6.32	126.81	119.47
1	B	138	GLN	C-N-CA	6.32	126.81	119.47
1	C	7	LEU	N-CA-C	6.24	119.63	109.59
1	B	123	GLN	N-CA-C	5.98	117.33	108.60
1	A	112	GLY	N-CA-C	-5.94	107.94	115.31
1	B	102	VAL	N-CA-C	5.86	117.19	109.21
1	A	135	GLU	N-CA-C	-5.60	105.58	113.20
1	B	157	ILE	N-CA-C	5.58	116.10	107.78
1	B	7	LEU	N-CA-C	5.47	117.87	109.07
1	B	55	ASN	N-CA-C	5.37	119.39	112.41
1	B	143	ASP	N-CA-C	5.30	115.03	108.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ASP	N-CA-C	5.24	115.15	108.24
1	C	55	ASN	N-CA-C	5.18	119.15	112.41
1	A	109	LYS	N-CA-C	-5.14	107.01	113.28
1	B	149	ASP	N-CA-C	-5.00	106.96	113.16

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	1270	0	1299	188	0
1	B	1412	0	1454	168	0
1	C	1412	0	1454	160	0
All	All	4094	0	4207	476	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 57.

All (476) 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:138:GLN:HE22	1:A:140:ARG:HB2	1.06	1.09
1:B:138:GLN:HB2	1:B:149:ASP:HB2	1.34	1.08
1:A:123:GLN:CD	1:A:124:THR:H	1.67	1.02
1:A:14:VAL:HG22	1:A:15:THR:H	1.23	1.01
1:A:77:THR:HB	1:A:129:ILE:HD13	1.38	1.00
1:A:138:GLN:NE2	1:A:140:ARG:HB2	1.76	1.00
1:C:12:ARG:HH11	1:C:12:ARG:HB3	1.25	1.00
1:A:114:GLN:HA	1:A:114:GLN:HE21	1.31	0.95
1:B:67:ARG:HH11	1:B:67:ARG:HG2	1.31	0.95
1:C:138:GLN:HB2	1:C:149:ASP:HB2	1.49	0.94
1:B:20:LEU:HD23	1:B:145:ILE:HD13	1.48	0.92
1:B:7:LEU:HD12	1:B:7:LEU:H	1.33	0.90
1:B:118:ILE:HD12	1:B:118:ILE:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:HE3	1:B:184:ILE:HD11	1.54	0.88
1:A:85:PRO:HA	1:A:121:ALA:HA	1.55	0.87
1:A:119:GLY:C	1:A:121:ALA:H	1.84	0.86
1:B:18:THR:HA	1:C:22:ALA:HA	1.55	0.86
1:A:49:ALA:HB3	1:A:155:ILE:HB	1.56	0.86
1:A:138:GLN:HE22	1:A:140:ARG:CB	1.88	0.85
1:A:12:ARG:HB2	1:A:12:ARG:NH1	1.94	0.83
1:C:90:THR:HB	1:C:158:THR:HB	1.58	0.83
1:A:77:THR:HB	1:A:129:ILE:CD1	2.08	0.83
1:A:103:THR:O	1:A:106:GLN:HG2	1.79	0.82
1:B:20:LEU:HD22	1:C:20:LEU:HD21	1.61	0.82
1:A:12:ARG:HB2	1:A:12:ARG:HH11	1.42	0.81
1:B:51:LEU:HD13	1:B:51:LEU:H	1.45	0.81
1:C:13:THR:HG22	1:C:136:MET:HE3	1.62	0.80
1:A:84:ALA:HB1	1:A:119:GLY:CA	2.11	0.80
1:B:148:LEU:HD21	1:C:145:ILE:HA	1.66	0.77
1:A:67:ARG:NH2	1:C:17:ALA:HB2	2.00	0.76
1:A:78:ILE:HG13	1:A:128:LEU:HB2	1.68	0.76
1:A:67:ARG:HH22	1:C:17:ALA:HB2	1.51	0.76
1:A:53:ILE:C	1:A:53:ILE:HD12	2.11	0.76
1:B:138:GLN:HE22	1:B:140:ARG:HB2	1.51	0.75
1:B:103:THR:O	1:B:106:GLN:HG2	1.85	0.75
1:C:53:ILE:HG23	1:C:56:ILE:HD11	1.69	0.75
1:C:12:ARG:HH11	1:C:12:ARG:CB	1.99	0.74
1:A:99:GLN:HG2	1:A:149:ASP:HA	1.70	0.74
1:C:13:THR:HG22	1:C:136:MET:CE	2.18	0.74
1:A:84:ALA:HB3	1:A:85:PRO:HD3	1.71	0.73
1:B:37:SER:HB3	1:B:58:SER:OG	1.88	0.73
1:A:84:ALA:HB1	1:A:119:GLY:HA3	1.71	0.73
1:A:15:THR:HG23	1:B:29:LEU:HD23	1.71	0.72
1:B:67:ARG:HH11	1:B:67:ARG:CG	2.01	0.72
1:A:31:ILE:HD12	1:A:31:ILE:H	1.54	0.72
1:A:78:ILE:HG22	1:A:171:ILE:HG12	1.72	0.72
1:B:20:LEU:HD13	1:B:21:PRO:HD2	1.72	0.71
1:B:95:TRP:CE2	1:B:132:CYS:HB2	2.25	0.71
1:A:15:THR:HG21	1:B:29:LEU:HB2	1.72	0.71
1:B:87:PHE:CG	1:B:164:PRO:HB3	2.26	0.71
1:A:78:ILE:CG2	1:A:171:ILE:HG12	2.20	0.71
1:B:20:LEU:HA	1:C:20:LEU:HD22	1.73	0.71
1:B:15:THR:HG23	1:C:181:SER:HB3	1.72	0.70
1:C:76:VAL:HG23	1:C:130:VAL:HB	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG22	1:A:15:THR:N	2.04	0.69
1:C:51:LEU:CD2	1:C:153:LEU:HB3	2.22	0.69
1:C:160:GLN:HG3	1:C:161:PRO:HD2	1.73	0.69
1:A:45:LYS:HB2	1:A:45:LYS:NZ	2.08	0.69
1:A:38:GLU:HA	1:A:172:THR:HG22	1.72	0.69
1:B:138:GLN:NE2	1:B:140:ARG:HB2	2.08	0.69
1:B:82:LEU:H	1:B:82:LEU:HD23	1.58	0.69
1:A:88:PRO:HA	1:A:119:GLY:O	1.94	0.68
1:A:135:GLU:CD	1:A:135:GLU:H	2.01	0.68
1:C:88:PRO:HG3	1:C:120:GLY:HA3	1.74	0.68
1:B:145:ILE:HD11	1:B:147:TYR:CE1	2.27	0.68
1:A:118:ILE:HG21	1:A:169:CYS:HB3	1.77	0.67
1:C:87:PHE:CG	1:C:164:PRO:HB3	2.28	0.67
1:B:5:LYS:NZ	1:B:5:LYS:HB3	2.10	0.67
1:C:42:ALA:HB1	1:C:157:ILE:HG21	1.76	0.67
1:B:118:ILE:HD12	1:B:118:ILE:N	2.09	0.67
1:A:29:LEU:HD12	1:A:29:LEU:H	1.58	0.67
1:C:132:CYS:SG	1:C:137:MET:HE3	2.35	0.67
1:C:87:PHE:O	1:C:89:THR:HG22	1.94	0.67
1:A:138:GLN:HB2	1:A:149:ASP:OD1	1.94	0.66
1:B:52:THR:HG22	1:B:54:ALA:H	1.59	0.66
1:C:95:TRP:CE2	1:C:132:CYS:HB2	2.30	0.66
1:A:51:LEU:HD12	1:A:153:LEU:HB3	1.76	0.66
1:A:145:ILE:HD12	1:B:145:ILE:HG21	1.78	0.66
1:A:120:GLY:N	1:A:123:GLN:HG2	2.10	0.66
1:A:40:LEU:HD23	1:A:171:ILE:HD12	1.77	0.66
1:B:98:ALA:HA	1:B:152:LYS:HE3	1.77	0.66
1:A:160:GLN:OE1	1:A:161:PRO:HD2	1.96	0.65
1:B:45:LYS:HB2	1:B:45:LYS:NZ	2.11	0.65
1:B:31:ILE:HD12	1:B:31:ILE:H	1.61	0.65
1:C:99:GLN:HG2	1:C:149:ASP:HA	1.78	0.65
1:A:39:VAL:HG22	1:A:51:LEU:HD22	1.79	0.65
1:A:134:LEU:C	1:A:136:MET:H	2.04	0.65
1:B:71:LEU:HD23	1:B:177:LEU:HD23	1.80	0.64
1:C:102:VAL:HG23	1:C:154:LEU:HD11	1.79	0.64
1:A:51:LEU:CD1	1:A:153:LEU:HB3	2.27	0.64
1:B:13:THR:HG22	1:B:136:MET:HE3	1.79	0.64
1:A:116:PHE:CG	1:A:128:LEU:HD13	2.33	0.64
1:C:88:PRO:HG3	1:C:120:GLY:CA	2.28	0.64
1:C:138:GLN:HG3	1:C:149:ASP:OD1	1.98	0.64
1:A:82:LEU:O	1:A:85:PRO:HD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLN:HG3	1:B:161:PRO:HD2	1.80	0.63
1:A:35:PHE:CD1	1:A:35:PHE:C	2.76	0.63
1:C:67:ARG:CB	1:C:67:ARG:HH11	2.12	0.63
1:C:51:LEU:HD23	1:C:153:LEU:HB3	1.79	0.63
1:A:95:TRP:CE2	1:A:132:CYS:HB2	2.33	0.63
1:A:123:GLN:O	1:A:124:THR:HG22	1.99	0.63
1:C:80:PRO:HG3	1:C:118:ILE:HG23	1.81	0.62
1:A:27:SER:HB3	1:A:28:PRO:HD3	1.82	0.62
1:B:118:ILE:H	1:B:118:ILE:CD1	2.10	0.62
1:A:87:PHE:CD2	1:A:164:PRO:HB3	2.35	0.62
1:B:19:VAL:CG2	1:B:140:ARG:HG3	2.30	0.62
1:A:122:ILE:O	1:A:122:ILE:CG2	2.48	0.61
1:C:160:GLN:CG	1:C:161:PRO:HD2	2.29	0.61
1:C:183:LEU:CD1	1:C:185:THR:HB	2.31	0.61
1:A:120:GLY:H	1:A:123:GLN:HG2	1.64	0.61
1:B:129:ILE:HD12	1:B:129:ILE:N	2.16	0.61
1:A:96:VAL:CG1	1:A:100:SER:HB3	2.31	0.61
1:C:72:GLU:HA	1:C:72:GLU:OE1	2.01	0.61
1:A:52:THR:HA	1:A:152:LYS:HA	1.82	0.60
1:A:119:GLY:O	1:A:121:ALA:N	2.34	0.60
1:B:51:LEU:HD13	1:B:51:LEU:N	2.17	0.60
1:C:183:LEU:HD13	1:C:183:LEU:C	2.26	0.60
1:A:122:ILE:O	1:A:122:ILE:HG23	2.01	0.60
1:C:54:ALA:HA	1:C:141:VAL:CG2	2.32	0.60
1:A:90:THR:HB	1:A:158:THR:OG1	2.01	0.60
1:A:144:SER:O	1:C:148:LEU:HG	2.01	0.60
1:A:52:THR:O	1:A:54:ALA:N	2.35	0.60
1:A:69:ALA:HB3	1:A:142:LYS:HB3	1.84	0.60
1:A:84:ALA:HB1	1:A:119:GLY:HA2	1.82	0.60
1:B:20:LEU:HD22	1:C:20:LEU:CD2	2.30	0.60
1:C:183:LEU:HD12	1:C:185:THR:HB	1.83	0.60
1:A:88:PRO:HG3	1:A:121:ALA:HB2	1.82	0.59
1:B:160:GLN:CG	1:B:161:PRO:HD2	2.32	0.59
1:C:6:GLU:C	1:C:7:LEU:HD12	2.27	0.59
1:B:51:LEU:HD22	1:B:153:LEU:HB3	1.82	0.59
1:C:102:VAL:CG2	1:C:154:LEU:HD11	2.32	0.59
1:A:85:PRO:HG3	1:A:123:GLN:NE2	2.18	0.59
1:A:119:GLY:C	1:A:121:ALA:N	2.52	0.59
1:C:5:LYS:HB3	1:C:129:ILE:HD11	1.85	0.59
1:A:148:LEU:HG	1:B:144:SER:O	2.02	0.59
1:A:39:VAL:HG13	1:A:51:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TRP:CD1	1:A:129:ILE:HG23	2.37	0.59
1:A:117:CYS:O	1:A:118:ILE:C	2.45	0.59
1:B:15:THR:OG1	1:C:182:PRO:HD2	2.02	0.59
1:A:87:PHE:CE2	1:A:165:PRO:HD3	2.38	0.58
1:C:17:ALA:HB1	1:C:138:GLN:HG2	1.85	0.58
1:A:45:LYS:HB2	1:A:45:LYS:HZ2	1.68	0.58
1:A:30:THR:HG22	1:A:180:HIS:HB3	1.85	0.58
1:A:75:TRP:CD1	1:A:129:ILE:HD12	2.38	0.58
1:B:90:THR:HB	1:B:158:THR:OG1	2.04	0.58
1:A:53:ILE:HD11	1:A:71:LEU:HD11	1.85	0.58
1:B:6:GLU:O	1:B:128:LEU:HA	2.04	0.58
1:B:98:ALA:HA	1:B:152:LYS:HB2	1.85	0.58
1:B:94:CYS:HB2	1:B:113:GLY:HA2	1.86	0.58
1:B:148:LEU:HD23	1:B:148:LEU:N	2.18	0.58
1:C:67:ARG:HD2	1:C:183:LEU:HD23	1.85	0.58
1:A:144:SER:HB2	1:C:18:THR:HB	1.85	0.57
1:B:60:SER:O	1:B:64:THR:HG23	2.04	0.57
1:C:44:THR:HA	1:C:164:PRO:HD2	1.86	0.57
1:B:12:ARG:HB2	1:B:136:MET:SD	2.44	0.57
1:B:87:PHE:CD1	1:B:164:PRO:HB3	2.39	0.57
1:A:65:PHE:CE1	1:A:187:THR:HG22	2.40	0.57
1:C:87:PHE:CD2	1:C:164:PRO:HB3	2.39	0.57
1:B:160:GLN:CD	1:B:161:PRO:HD2	2.30	0.57
1:C:7:LEU:HD12	1:C:7:LEU:N	2.19	0.57
1:A:51:LEU:HD12	1:A:51:LEU:O	2.05	0.57
1:B:81:THR:HG23	1:B:169:CYS:HA	1.86	0.57
1:A:78:ILE:HD11	1:A:116:PHE:CD2	2.40	0.57
1:A:149:ASP:CG	1:B:67:ARG:HH12	2.13	0.57
1:A:76:VAL:CG1	1:A:130:VAL:HB	2.35	0.56
1:A:86:THR:HG23	1:A:87:PHE:CD2	2.40	0.56
1:A:88:PRO:O	1:A:160:GLN:HG2	2.05	0.56
1:B:16:VAL:HG22	1:C:181:SER:OG	2.06	0.56
1:B:19:VAL:HG23	1:B:147:TYR:CZ	2.41	0.56
1:B:7:LEU:HD12	1:B:7:LEU:N	2.08	0.56
1:B:40:LEU:HD12	1:B:155:ILE:HG21	1.88	0.56
1:C:123:GLN:O	1:C:123:GLN:HG3	2.06	0.56
1:C:137:MET:HG2	1:C:151:PRO:HG3	1.87	0.56
1:A:149:ASP:CB	1:B:67:ARG:NH1	2.69	0.56
1:C:134:LEU:H	1:C:134:LEU:HD22	1.71	0.55
1:C:135:GLU:H	1:C:135:GLU:CD	2.14	0.55
1:A:123:GLN:CD	1:A:124:THR:N	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLN:HE22	1:C:140:ARG:HB2	1.71	0.55
1:B:42:ALA:HB3	1:B:157:ILE:HD13	1.89	0.55
1:B:146:GLN:O	1:B:146:GLN:HG3	2.05	0.55
1:A:114:GLN:HA	1:A:114:GLN:NE2	2.12	0.55
1:A:133:PRO:O	1:A:137:MET:HE3	2.05	0.55
1:A:181:SER:HB3	1:C:15:THR:HG23	1.89	0.55
1:C:123:GLN:O	1:C:123:GLN:CG	2.55	0.55
1:C:143:ASP:CG	1:C:144:SER:H	2.15	0.55
1:B:19:VAL:HG11	1:C:23:VAL:HG12	1.89	0.55
1:B:31:ILE:HD12	1:B:179:MET:O	2.07	0.55
1:C:138:GLN:HB2	1:C:149:ASP:CB	2.32	0.55
1:A:145:ILE:CD1	1:B:20:LEU:HD21	2.37	0.54
1:A:51:LEU:HD11	1:A:153:LEU:HD23	1.88	0.54
1:B:19:VAL:HG21	1:B:140:ARG:HG3	1.88	0.54
1:B:32:LYS:HA	1:B:177:LEU:O	2.07	0.54
1:C:31:ILE:HD12	1:C:31:ILE:H	1.71	0.54
1:B:138:GLN:C	1:B:138:GLN:OE1	2.51	0.54
1:C:160:GLN:CD	1:C:161:PRO:HD2	2.33	0.54
1:A:95:TRP:CD1	1:A:132:CYS:HA	2.43	0.54
1:A:99:GLN:HG2	1:A:149:ASP:CA	2.36	0.54
1:C:138:GLN:NE2	1:C:140:ARG:HB2	2.23	0.54
1:B:20:LEU:HB2	1:B:147:TYR:OH	2.08	0.54
1:B:135:GLU:CD	1:B:135:GLU:H	2.15	0.54
1:B:120:GLY:O	1:B:122:ILE:N	2.40	0.54
1:C:5:LYS:HB3	1:C:129:ILE:CD1	2.37	0.54
1:C:5:LYS:HD2	1:C:5:LYS:N	2.22	0.54
1:B:82:LEU:HD23	1:B:82:LEU:N	2.23	0.53
1:C:85:PRO:HG3	1:C:125:LEU:HD21	1.90	0.53
1:A:32:LYS:HA	1:A:177:LEU:O	2.08	0.53
1:C:54:ALA:HB2	1:C:150:SER:OG	2.07	0.53
1:C:122:ILE:HD13	1:C:123:GLN:H	1.73	0.53
1:A:94:CYS:HB2	1:A:107:ILE:HG23	1.89	0.53
1:B:138:GLN:HB2	1:B:149:ASP:CB	2.23	0.53
1:B:12:ARG:HG2	1:B:12:ARG:HH11	1.73	0.53
1:A:91:VAL:HG11	1:A:118:ILE:CG1	2.38	0.53
1:C:13:THR:N	1:C:136:MET:HE3	2.24	0.53
1:A:72:GLU:HB2	1:A:176:THR:HB	1.91	0.53
1:B:75:TRP:HB2	1:B:131:LYS:HA	1.91	0.53
1:B:107:ILE:HG23	1:B:113:GLY:HA3	1.91	0.53
1:A:180:HIS:O	1:A:181:SER:HB2	2.09	0.52
1:A:185:THR:HA	1:C:102:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:CG2	1:B:29:LEU:HB2	2.38	0.52
1:B:23:VAL:HG23	1:B:24:PRO:HD2	1.91	0.52
1:B:95:TRP:CD2	1:B:132:CYS:HB2	2.43	0.52
1:B:103:THR:HG23	1:B:106:GLN:HG2	1.92	0.52
1:C:33:GLN:HG2	1:C:62:LEU:HD22	1.91	0.52
1:C:51:LEU:HD21	1:C:153:LEU:HB3	1.92	0.52
1:A:15:THR:CG2	1:B:29:LEU:H	2.23	0.52
1:A:31:ILE:HD12	1:A:31:ILE:N	2.24	0.52
1:B:44:THR:HA	1:B:164:PRO:HD2	1.92	0.52
1:C:86:THR:HG23	1:C:87:PHE:CD2	2.45	0.52
1:C:96:VAL:HG12	1:C:100:SER:HB3	1.92	0.52
1:C:39:VAL:HB	1:C:171:ILE:HG22	1.90	0.52
1:C:53:ILE:O	1:C:56:ILE:HG13	2.09	0.52
1:A:43:GLY:HA3	1:A:168:THR:OG1	2.10	0.52
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.75	0.52
1:C:32:LYS:HA	1:C:177:LEU:O	2.10	0.51
1:A:77:THR:HA	1:A:128:LEU:O	2.10	0.51
1:B:85:PRO:HG3	1:B:125:LEU:HD11	1.92	0.51
1:A:106:GLN:HB2	1:A:109:LYS:HD2	1.92	0.51
1:A:14:VAL:CG2	1:A:15:THR:H	2.05	0.51
1:C:53:ILE:HG13	1:C:74:LEU:HD21	1.93	0.51
1:A:53:ILE:HG21	1:A:95:TRP:CH2	2.46	0.51
1:A:149:ASP:OD2	1:B:144:SER:HA	2.10	0.51
1:B:12:ARG:NH2	1:B:133:PRO:HB3	2.26	0.51
1:A:97:PRO:HG2	1:B:183:LEU:HD23	1.92	0.51
1:A:143:ASP:CG	1:A:144:SER:H	2.18	0.51
1:C:133:PRO:HA	1:C:135:GLU:OE1	2.11	0.51
1:A:52:THR:C	1:A:54:ALA:N	2.68	0.51
1:B:92:GLY:HA2	1:B:115:ILE:HA	1.92	0.51
1:A:75:TRP:NE1	1:A:129:ILE:HD12	2.26	0.50
1:C:74:LEU:HD23	1:C:132:CYS:SG	2.52	0.50
1:C:89:THR:HG21	1:C:168:THR:OG1	2.10	0.50
1:A:53:ILE:HD12	1:A:54:ALA:N	2.26	0.50
1:B:51:LEU:CD2	1:B:153:LEU:HB3	2.41	0.50
1:B:116:PHE:HB2	1:B:118:ILE:HD11	1.94	0.50
1:C:103:THR:HG23	1:C:106:GLN:HG3	1.92	0.50
1:B:54:ALA:HA	1:B:141:VAL:CG2	2.42	0.50
1:A:138:GLN:O	1:A:151:PRO:HD3	2.12	0.50
1:C:96:VAL:CG1	1:C:97:PRO:HD2	2.41	0.50
1:C:128:LEU:C	1:C:129:ILE:HG13	2.36	0.50
1:A:118:ILE:HG21	1:A:169:CYS:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ALA:O	1:C:23:VAL:HG13	2.12	0.50
1:B:99:GLN:HG2	1:B:149:ASP:HA	1.93	0.50
1:B:145:ILE:HD12	1:C:145:ILE:HG21	1.94	0.49
1:A:109:LYS:HB3	1:B:186:ASP:OD1	2.13	0.49
1:A:134:LEU:C	1:A:136:MET:N	2.68	0.49
1:B:12:ARG:HH21	1:B:133:PRO:HB3	1.77	0.49
1:B:38:GLU:HA	1:B:172:THR:HG22	1.94	0.49
1:A:95:TRP:CD2	1:A:132:CYS:HB2	2.46	0.49
1:B:5:LYS:O	1:B:5:LYS:HG3	2.12	0.49
1:C:29:LEU:N	1:C:29:LEU:HD12	2.28	0.49
1:C:74:LEU:O	1:C:75:TRP:HB3	2.13	0.49
1:A:31:ILE:CD1	1:A:179:MET:HB2	2.41	0.49
1:B:75:TRP:CB	1:B:131:LYS:HA	2.42	0.49
1:B:128:LEU:HD23	1:B:129:ILE:N	2.27	0.49
1:C:95:TRP:CD2	1:C:132:CYS:HB2	2.47	0.49
1:B:5:LYS:HB3	1:B:5:LYS:HZ3	1.77	0.49
1:C:67:ARG:HH11	1:C:67:ARG:HB2	1.76	0.49
1:C:95:TRP:CD1	1:C:132:CYS:HA	2.48	0.49
1:C:137:MET:CG	1:C:151:PRO:HG3	2.43	0.49
1:B:67:ARG:CG	1:B:67:ARG:NH1	2.67	0.49
1:A:52:THR:C	1:A:54:ALA:H	2.19	0.49
1:A:71:LEU:HD23	1:A:177:LEU:HD23	1.95	0.49
1:A:104:PRO:C	1:A:106:GLN:H	2.20	0.49
1:C:29:LEU:O	1:C:180:HIS:HB2	2.12	0.49
1:A:76:VAL:HG12	1:A:130:VAL:HB	1.95	0.49
1:B:41:PHE:CE1	1:B:170:ILE:HG12	2.48	0.49
1:A:116:PHE:CE1	1:A:128:LEU:HD22	2.48	0.48
1:B:102:VAL:HG12	1:B:154:LEU:HD21	1.95	0.48
1:B:61:THR:HA	1:B:64:THR:HG23	1.95	0.48
1:B:80:PRO:HG3	1:B:118:ILE:HG23	1.94	0.48
1:C:80:PRO:HG3	1:C:118:ILE:CG2	2.43	0.48
1:C:122:ILE:HD13	1:C:123:GLN:N	2.28	0.48
1:C:138:GLN:OE1	1:C:138:GLN:C	2.55	0.48
1:A:74:LEU:HD23	1:A:132:CYS:SG	2.53	0.48
1:A:163:ALA:HA	1:A:164:PRO:HD3	1.72	0.48
1:B:97:PRO:C	1:B:99:GLN:N	2.70	0.48
1:A:179:MET:O	1:A:180:HIS:HB3	2.13	0.48
1:A:85:PRO:HG3	1:A:123:GLN:HE21	1.78	0.48
1:B:31:ILE:HD13	1:B:179:MET:HE3	1.95	0.48
1:C:96:VAL:CG1	1:C:100:SER:HB3	2.44	0.48
1:B:137:MET:HG3	1:B:151:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HG11	1:A:118:ILE:HG12	1.95	0.47
1:B:86:THR:HB	1:B:87:PHE:CD1	2.49	0.47
1:A:110:THR:HG22	1:A:111:TYR:N	2.29	0.47
1:B:69:ALA:HB3	1:B:142:LYS:HB3	1.96	0.47
1:C:188:SER:O	1:C:189:THR:HG23	2.13	0.47
1:B:7:LEU:N	1:B:7:LEU:CD1	2.72	0.47
1:B:83:GLN:HB3	1:B:168:THR:HG22	1.95	0.47
1:B:52:THR:HG22	1:B:54:ALA:HB3	1.95	0.47
1:C:32:LYS:NZ	1:C:32:LYS:HB3	2.29	0.47
1:B:20:LEU:HD23	1:B:145:ILE:CD1	2.33	0.47
1:C:107:ILE:O	1:C:113:GLY:HA3	2.14	0.47
1:A:183:LEU:HD11	1:C:100:SER:HB2	1.96	0.47
1:A:120:GLY:O	1:A:121:ALA:O	2.32	0.47
1:A:53:ILE:HG21	1:A:95:TRP:HH2	1.78	0.47
1:A:149:ASP:HB2	1:B:67:ARG:NH1	2.30	0.47
1:C:4:ASP:O	1:C:127:PRO:HD2	2.14	0.47
1:C:35:PHE:CD1	1:C:35:PHE:C	2.93	0.47
1:C:75:TRP:CB	1:C:131:LYS:HA	2.45	0.47
1:C:102:VAL:HG23	1:C:154:LEU:CD1	2.44	0.47
1:C:122:ILE:O	1:C:123:GLN:HB3	2.15	0.47
1:A:41:PHE:CE1	1:A:170:ILE:HG12	2.50	0.47
1:A:57:ASP:CG	1:A:58:SER:H	2.23	0.47
1:C:94:CYS:HB2	1:C:113:GLY:HA2	1.97	0.47
1:B:53:ILE:HD12	1:B:173:VAL:HG11	1.97	0.46
1:A:53:ILE:CD1	1:A:71:LEU:HD11	2.45	0.46
1:A:118:ILE:HD11	1:A:128:LEU:HD12	1.97	0.46
1:C:187:THR:O	1:C:188:SER:C	2.59	0.46
1:A:83:GLN:O	1:A:84:ALA:C	2.58	0.46
1:B:15:THR:HG21	1:C:67:ARG:HE	1.80	0.46
1:C:92:GLY:HA2	1:C:114:GLN:O	2.14	0.46
1:C:161:PRO:HG2	1:C:162:THR:H	1.80	0.46
1:A:44:THR:HA	1:A:164:PRO:HD2	1.96	0.46
1:B:6:GLU:O	1:B:129:ILE:HD12	2.15	0.46
1:C:97:PRO:O	1:C:99:GLN:N	2.49	0.46
1:C:138:GLN:NE2	1:C:147:TYR:CG	2.83	0.46
1:A:124:THR:O	1:A:125:LEU:CB	2.63	0.46
1:A:135:GLU:CD	1:A:135:GLU:N	2.72	0.46
1:B:10:GLN:HA	1:B:114:GLN:HE22	1.80	0.46
1:B:54:ALA:HA	1:B:141:VAL:HG22	1.98	0.46
1:A:138:GLN:NE2	1:A:147:TYR:CD2	2.83	0.46
1:A:87:PHE:O	1:A:88:PRO:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ALA:CB	1:C:157:ILE:HG13	2.45	0.46
1:B:116:PHE:CD1	1:B:128:LEU:HD11	2.51	0.46
1:C:97:PRO:C	1:C:99:GLN:N	2.74	0.46
1:A:184:ILE:HG22	1:C:110:THR:HG23	1.98	0.45
1:A:93:VAL:HA	1:A:154:LEU:O	2.15	0.45
1:A:185:THR:OG1	1:C:101:PRO:HG2	2.16	0.45
1:B:51:LEU:HD22	1:B:51:LEU:O	2.16	0.45
1:C:49:ALA:HB3	1:C:155:ILE:HB	1.98	0.45
1:C:19:VAL:CG1	1:C:140:ARG:CZ	2.94	0.45
1:B:35:PHE:CD1	1:B:35:PHE:C	2.94	0.45
1:C:54:ALA:HA	1:C:141:VAL:HG23	1.98	0.45
1:B:82:LEU:H	1:B:82:LEU:CD2	2.26	0.45
1:C:7:LEU:N	1:C:7:LEU:CD1	2.80	0.45
1:B:19:VAL:HG23	1:B:140:ARG:HG3	1.99	0.45
1:C:87:PHE:CZ	1:C:164:PRO:HA	2.52	0.45
1:C:145:ILE:HD11	1:C:147:TYR:CZ	2.51	0.45
1:C:148:LEU:C	1:C:150:SER:H	2.25	0.45
1:B:45:LYS:HB2	1:B:45:LYS:HZ2	1.82	0.45
1:B:143:ASP:CG	1:B:144:SER:H	2.25	0.45
1:C:67:ARG:HD3	1:C:183:LEU:HA	1.97	0.45
1:C:88:PRO:O	1:C:160:GLN:NE2	2.51	0.45
1:C:183:LEU:O	1:C:185:THR:N	2.50	0.45
1:A:96:VAL:HG13	1:A:97:PRO:HD2	1.99	0.44
1:B:39:VAL:HG12	1:B:171:ILE:O	2.16	0.44
1:C:41:PHE:CE1	1:C:170:ILE:HG23	2.52	0.44
1:A:71:LEU:HD23	1:A:177:LEU:CD2	2.46	0.44
1:B:77:THR:HG23	1:B:79:HIS:HE1	1.82	0.44
1:A:39:VAL:HG22	1:A:51:LEU:CD2	2.46	0.44
1:A:101:PRO:HG2	1:B:185:THR:OG1	2.17	0.44
1:A:111:TYR:C	1:A:113:GLY:H	2.25	0.44
1:B:84:ALA:HB3	1:B:85:PRO:HD3	1.99	0.44
1:C:53:ILE:HG23	1:C:56:ILE:CD1	2.45	0.44
1:A:87:PHE:CZ	1:A:165:PRO:HD3	2.52	0.44
1:B:180:HIS:O	1:B:181:SER:HB3	2.18	0.44
1:B:153:LEU:HD22	1:B:154:LEU:N	2.32	0.44
1:A:51:LEU:O	1:A:153:LEU:N	2.45	0.44
1:A:104:PRO:C	1:A:106:GLN:N	2.76	0.44
1:A:124:THR:O	1:A:125:LEU:HB2	2.17	0.44
1:C:155:ILE:CD1	1:C:171:ILE:HG21	2.47	0.44
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.79	0.44
1:B:8:ALA:HA	1:B:9:PRO:HD2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PHE:O	1:B:174:SER:HA	2.18	0.44
1:C:96:VAL:HG13	1:C:97:PRO:HD2	2.00	0.44
1:C:112:GLY:O	1:C:113:GLY:C	2.60	0.44
1:C:147:TYR:C	1:C:148:LEU:HD23	2.42	0.44
1:A:123:GLN:OE1	1:A:124:THR:N	2.46	0.43
1:B:8:ALA:HB3	1:B:128:LEU:HD21	2.00	0.43
1:B:185:THR:HG23	1:B:186:ASP:N	2.33	0.43
1:C:133:PRO:C	1:C:135:GLU:N	2.74	0.43
1:C:83:GLN:HB3	1:C:168:THR:HG22	2.00	0.43
1:A:30:THR:HG22	1:A:180:HIS:CB	2.48	0.43
1:A:116:PHE:CD1	1:A:128:LEU:HD13	2.53	0.43
1:C:49:ALA:O	1:C:155:ILE:N	2.51	0.43
1:C:51:LEU:HD21	1:C:153:LEU:HD23	1.99	0.43
1:C:41:PHE:CE1	1:C:170:ILE:HG12	2.52	0.43
1:A:137:MET:O	1:A:139:PRO:HD3	2.18	0.43
1:B:41:PHE:CE1	1:B:170:ILE:HG23	2.54	0.43
1:B:52:THR:C	1:B:54:ALA:N	2.74	0.43
1:A:100:SER:HB2	1:B:183:LEU:HD21	2.00	0.43
1:B:18:THR:O	1:B:19:VAL:HB	2.18	0.43
1:B:138:GLN:NE2	1:B:147:TYR:CG	2.84	0.43
1:C:41:PHE:HE1	1:C:170:ILE:CD1	2.32	0.43
1:A:75:TRP:CB	1:A:131:LYS:HA	2.49	0.43
1:B:29:LEU:O	1:B:180:HIS:HB2	2.19	0.43
1:B:99:GLN:HB3	1:B:148:LEU:O	2.19	0.43
1:B:112:GLY:O	1:B:113:GLY:C	2.60	0.43
1:B:56:ILE:O	1:B:57:ASP:C	2.62	0.43
1:C:17:ALA:CB	1:C:138:GLN:HG2	2.49	0.43
1:B:103:THR:HG22	1:B:106:GLN:OE1	2.18	0.42
1:A:12:ARG:CG	1:A:13:THR:H	2.32	0.42
1:A:39:VAL:CG1	1:A:51:LEU:HD21	2.49	0.42
1:A:53:ILE:C	1:A:53:ILE:CD1	2.82	0.42
1:C:91:VAL:HG21	1:C:118:ILE:HG13	2.01	0.42
1:C:187:THR:C	1:C:189:THR:N	2.76	0.42
1:A:83:GLN:HA	1:A:83:GLN:NE2	2.34	0.42
1:B:45:LYS:HB2	1:B:45:LYS:HZ3	1.81	0.42
1:C:145:ILE:C	1:C:145:ILE:HD12	2.44	0.42
1:A:57:ASP:O	1:A:60:SER:HB3	2.19	0.42
1:B:77:THR:HG23	1:B:79:HIS:CE1	2.54	0.42
1:C:138:GLN:HA	1:C:139:PRO:HD2	1.78	0.42
1:B:31:ILE:HD12	1:B:31:ILE:N	2.30	0.42
1:A:133:PRO:HG2	1:A:137:MET:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:CG2	1:B:24:PRO:HD2	2.49	0.42
1:B:110:THR:O	1:B:111:TYR:C	2.63	0.42
1:B:19:VAL:HA	1:B:147:TYR:CE1	2.55	0.42
1:A:56:ILE:O	1:A:57:ASP:C	2.62	0.42
1:A:115:ILE:CG2	1:A:116:PHE:N	2.81	0.42
1:A:83:GLN:HA	1:A:83:GLN:HE21	1.85	0.42
1:A:86:THR:HG23	1:A:87:PHE:HD2	1.84	0.42
1:A:118:ILE:CD1	1:A:128:LEU:HD12	2.50	0.42
1:A:138:GLN:O	1:A:150:SER:HA	2.19	0.42
1:B:187:THR:O	1:B:188:SER:C	2.62	0.42
1:C:56:ILE:HG13	1:C:56:ILE:H	1.60	0.42
1:C:79:HIS:ND1	1:C:79:HIS:N	2.68	0.42
1:C:116:PHE:CD1	1:C:128:LEU:HD11	2.55	0.42
1:B:120:GLY:C	1:B:122:ILE:N	2.78	0.41
1:A:93:VAL:HG21	1:A:130:VAL:HG21	2.02	0.41
1:B:122:ILE:O	1:B:122:ILE:HG13	2.20	0.41
1:A:45:LYS:O	1:A:46:ASP:C	2.61	0.41
1:A:99:GLN:HE21	1:A:99:GLN:HB2	1.50	0.41
1:A:155:ILE:HG22	1:A:156:SER:N	2.36	0.41
1:A:81:THR:O	1:A:84:ALA:HB3	2.21	0.41
1:A:102:VAL:HG22	1:A:154:LEU:CD1	2.51	0.41
1:A:103:THR:HG23	1:A:106:GLN:OE1	2.20	0.41
1:A:145:ILE:HD11	1:B:20:LEU:HD21	2.01	0.41
1:C:106:GLN:O	1:C:107:ILE:C	2.64	0.41
1:A:51:LEU:HD11	1:A:153:LEU:HB3	2.01	0.41
1:B:119:GLY:C	1:B:123:GLN:NE2	2.79	0.41
1:C:138:GLN:NE2	1:C:147:TYR:CD1	2.88	0.41
1:C:52:THR:HG22	1:C:54:ALA:HB3	2.02	0.41
1:A:129:ILE:HG22	1:A:130:VAL:N	2.35	0.41
1:B:12:ARG:CB	1:B:136:MET:SD	3.07	0.41
1:A:57:ASP:O	1:A:61:THR:HG23	2.21	0.41
1:B:71:LEU:HD13	1:B:74:LEU:HG	2.03	0.41
1:B:138:GLN:HA	1:B:139:PRO:HD2	1.81	0.41
1:A:10:GLN:HG2	1:A:10:GLN:O	2.20	0.41
1:B:19:VAL:CG1	1:C:23:VAL:HG12	2.51	0.41
1:B:148:LEU:HG	1:C:144:SER:O	2.21	0.41
1:C:123:GLN:O	1:C:123:GLN:OE1	2.38	0.41
1:A:31:ILE:HD11	1:A:179:MET:HB2	2.03	0.41
1:A:42:ALA:CB	1:A:157:ILE:HG12	2.50	0.40
1:A:129:ILE:CG2	1:A:130:VAL:N	2.84	0.40
1:B:5:LYS:O	1:B:5:LYS:CG	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HB	1:B:87:PHE:CE1	2.56	0.40
1:C:128:LEU:HD23	1:C:128:LEU:HA	1.79	0.40
1:B:160:GLN:NE2	1:B:160:GLN:HA	2.37	0.40
1:C:43:GLY:HA3	1:C:168:THR:H	1.85	0.40
1:B:71:LEU:HD23	1:B:177:LEU:CD2	2.49	0.40
1:C:76:VAL:CG2	1:C:130:VAL:HB	2.47	0.40
1:B:97:PRO:C	1:B:99:GLN:H	2.26	0.40
1:C:75:TRP:CD1	1:C:129:ILE:HG23	2.57	0.40
1:B:37:SER:HB3	1:B:58:SER:CB	2.50	0.40
1:C:53:ILE:HA	1:C:56:ILE:HD11	2.04	0.40
1:C:75:TRP:HB2	1:C:131:LYS:HA	2.02	0.40
1:C:81:THR:HG23	1:C:169:CYS:HA	2.03	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	165/189 (87%)	121 (73%)	29 (18%)	15 (9%)	0	8
1	B	187/189 (99%)	146 (78%)	33 (18%)	8 (4%)	2	19
1	C	187/189 (99%)	157 (84%)	24 (13%)	6 (3%)	3	24
All	All	539/567 (95%)	424 (79%)	86 (16%)	29 (5%)	1	16

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	14	VAL
1	A	121	ALA
1	A	125	LEU
1	B	121	ALA

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Mol	Chain	Res	Type
1	A	53	ILE
1	A	57	ASP
1	A	118	ILE
1	B	57	ASP
1	B	113	GLY
1	C	113	GLY
1	C	184	ILE
1	A	12	ARG
1	B	111	TYR
1	C	98	ALA
1	A	98	ALA
1	A	149	ASP
1	A	181	SER
1	B	28	PRO
1	B	163	ALA
1	B	181	SER
1	C	140	ARG
1	C	163	ALA
1	C	181	SER
1	A	114	GLN
1	A	163	ALA
1	B	19	VAL
1	A	113	GLY
1	A	122	ILE

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	150/166 (90%)	129 (86%)	21 (14%)	3	18
1	B	166/166 (100%)	141 (85%)	25 (15%)	3	16
1	C	166/166 (100%)	141 (85%)	25 (15%)	3	16
All	All	482/498 (97%)	411 (85%)	71 (15%)	3	17

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	31	ILE
1	A	39	VAL
1	A	45	LYS
1	A	52	THR
1	A	77	THR
1	A	78	ILE
1	A	86	THR
1	A	99	GLN
1	A	102	VAL
1	A	103	THR
1	A	108	THR
1	A	114	GLN
1	A	115	ILE
1	A	122	ILE
1	A	124	THR
1	A	136	MET
1	A	138	GLN
1	A	148	LEU
1	A	149	ASP
1	A	181	SER
1	B	5	LYS
1	B	7	LEU
1	B	11	ASP
1	B	20	LEU
1	B	28	PRO
1	B	30	THR
1	B	31	ILE
1	B	39	VAL
1	B	45	LYS
1	B	51	LEU
1	B	67	ARG
1	B	74	LEU
1	B	83	GLN
1	B	103	THR
1	B	107	ILE
1	B	124	THR
1	B	129	ILE
1	B	138	GLN
1	B	141	VAL
1	B	148	LEU
1	B	149	ASP
1	B	153	LEU

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Mol	Chain	Res	Type
1	B	167	SER
1	B	183	LEU
1	B	185	THR
1	C	6	GLU
1	C	12	ARG
1	C	30	THR
1	C	31	ILE
1	C	41	PHE
1	C	61	THR
1	C	67	ARG
1	C	72	GLU
1	C	76	VAL
1	C	83	GLN
1	C	86	THR
1	C	89	THR
1	C	93	VAL
1	C	99	GLN
1	C	102	VAL
1	C	103	THR
1	C	122	ILE
1	C	125	LEU
1	C	138	GLN
1	C	141	VAL
1	C	145	ILE
1	C	149	ASP
1	C	167	SER
1	C	173	VAL
1	C	189	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	36	GLN
1	A	55	ASN
1	A	79	HIS
1	A	83	GLN
1	A	114	GLN
1	B	36	GLN
1	B	79	HIS
1	B	99	GLN
1	B	114	GLN

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Mol	Chain	Res	Type
1	B	160	GLN
1	C	55	ASN
1	C	99	GLN
1	C	146	GLN
1	C	160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	169/189 (89%)	0.70	25 (14%) 5 8	2, 38, 134, 140	0
1	B	189/189 (100%)	0.46	14 (7%) 20 18	0, 30, 97, 140	0
1	C	189/189 (100%)	0.39	9 (4%) 35 26	0, 31, 92, 136	0
All	All	547/567 (96%)	0.51	48 (8%) 15 15	0, 32, 104, 140	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	LEU	7.7
1	A	12	ARG	6.6
1	A	124	THR	6.0
1	C	189	THR	5.5
1	C	1	MET	5.2
1	A	14	VAL	5.0
1	C	25	GLY	4.7
1	A	27	SER	4.4
1	A	162	THR	4.3
1	A	122	ILE	4.2
1	B	25	GLY	4.2
1	B	1	MET	4.1
1	A	10	GLN	3.9
1	A	15	THR	3.8
1	A	123	GLN	3.7
1	C	2	GLU	3.7
1	C	43	GLY	3.5
1	B	186	ASP	3.3
1	B	24	PRO	3.3
1	A	43	GLY	3.2
1	A	189	THR	3.2
1	A	11	ASP	3.1
1	B	189	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	146	GLN	3.0
1	B	26	PRO	2.9
1	C	22	ALA	2.9
1	A	127	PRO	2.8
1	A	13	THR	2.8
1	A	126	SER	2.7
1	C	188	SER	2.7
1	B	175	GLY	2.7
1	B	109	LYS	2.6
1	C	146	GLN	2.6
1	B	2	GLU	2.4
1	A	119	GLY	2.3
1	B	23	VAL	2.3
1	A	48	GLU	2.3
1	B	72	GLU	2.3
1	A	45	LYS	2.2
1	C	123	GLN	2.2
1	A	28	PRO	2.2
1	B	161	PRO	2.2
1	B	167	SER	2.2
1	A	165	PRO	2.1
1	A	121	ALA	2.1
1	A	109	LYS	2.1
1	A	135	GLU	2.0
1	B	46	ASP	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.