



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 AM UTC

PDB ID : 8PEL / pdb_00008pel
Title : Structure of C. thermophilum RNA exosome core
Authors : Lazzaretti, D.; Holdermann, I.; Sprangers, R.
Deposited on : 2023-06-14
Resolution : 3.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

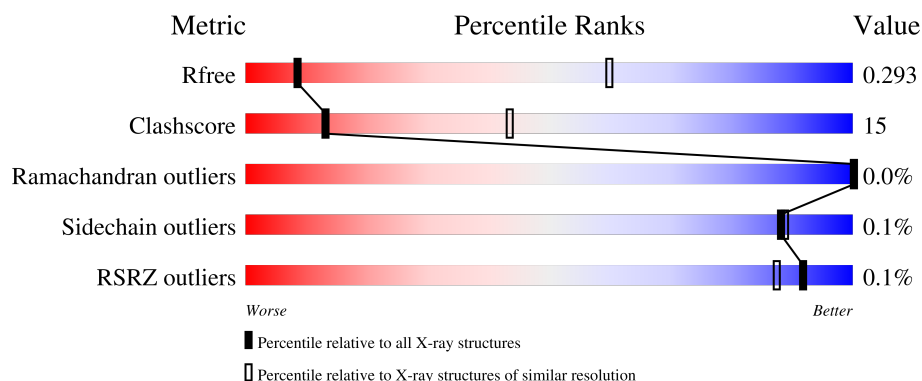
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

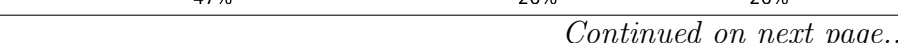
The reported resolution of this entry is 3.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)

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	293	 72% 24% .
2	B	284	 56% 19% 26%
3	C	357	 62% 25% 13%
4	D	258	 66% 24% 10%
5	E	413	 47% 26% 26%

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Mol	Chain	Length	Quality of chain
6	F	284	64% 31% 5%
7	G	256	64% 34%
8	H	358	53% 19% 27%
9	I	220	55% 26% 19%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 35554 atoms, of which 17898 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 Rrp45.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	H	N	O	S	4	0	0
			4376	1378	2195	375	417	11			

- Molecule 2 is a protein called Exoribonuclease phosphorolytic domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	211	Total	C	H	N	O	S	4	0	0
			3204	986	1610	290	307	11			

- Molecule 3 is a protein called Exoribonuclease-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	311	Total	C	H	N	O	S	0	0	0
			4939	1560	2490	435	445	9			

- Molecule 4 is a protein called Exoribonuclease phosphorolytic domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	232	Total	C	H	N	O	S	0	0	0
			3540	1117	1765	310	342	6			

- Molecule 5 is a protein called Exoribonuclease phosphorolytic domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	304	Total	C	H	N	O	S	0	0	0
			4726	1499	2393	395	436	3			

- Molecule 6 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	269	Total	C	H	N	O	S	3	0	0
			4068	1264	2040	359	393	12			

- Molecule 7 is a protein called Ribosomal RNA-processing protein 40.

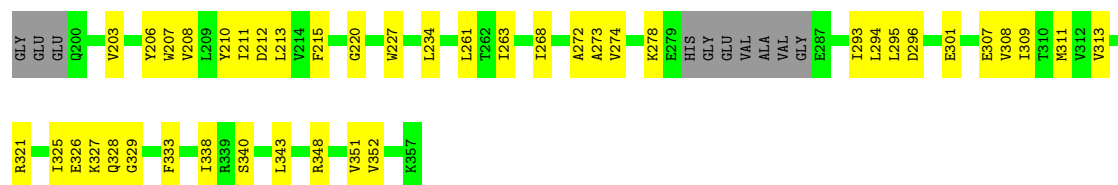
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	251	Total	C	H	N	O	S	0	0	0
			3897	1210	1971	353	355	8			

- Molecule 8 is a protein called Putative exosome complex protein.

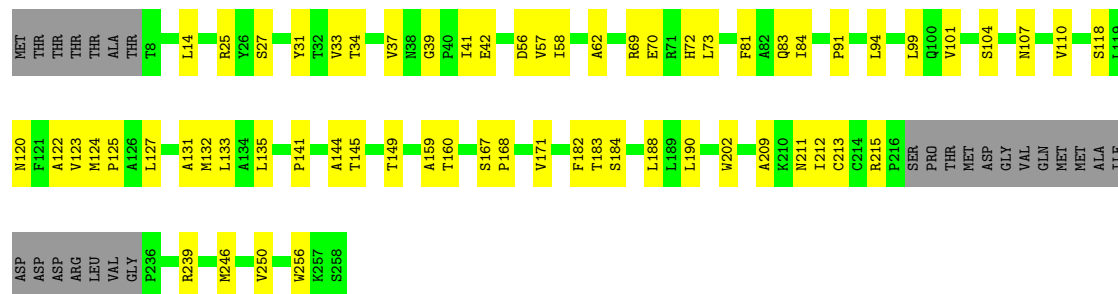
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	261	Total	C	H	N	O	S	0	0	0
			4013	1247	2020	362	376	8			

- Molecule 9 is a protein called Putative exosome 3'->5 protein.

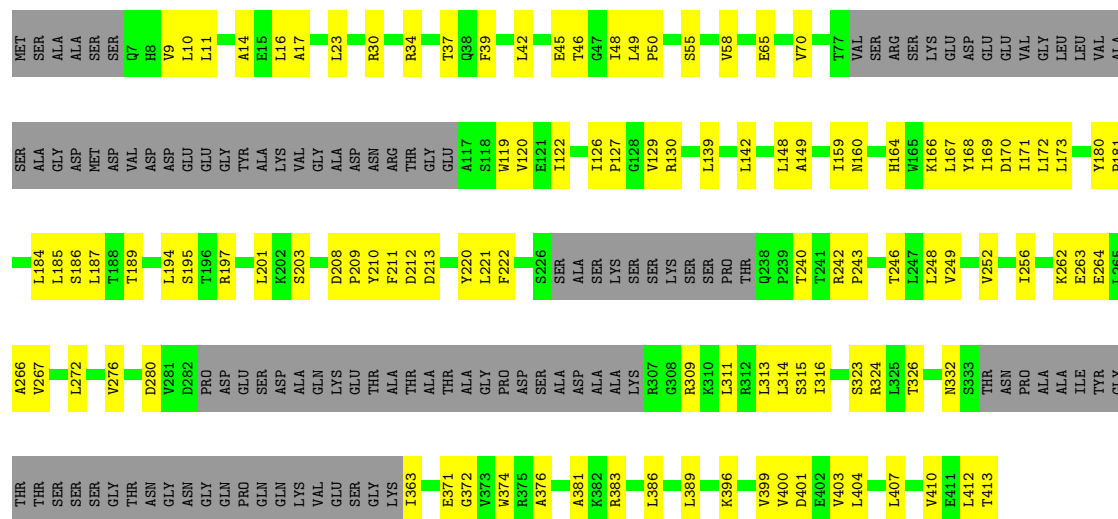
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	I	178	Total	C	H	N	O	S	0	0	0
			2791	872	1414	243	259	3			



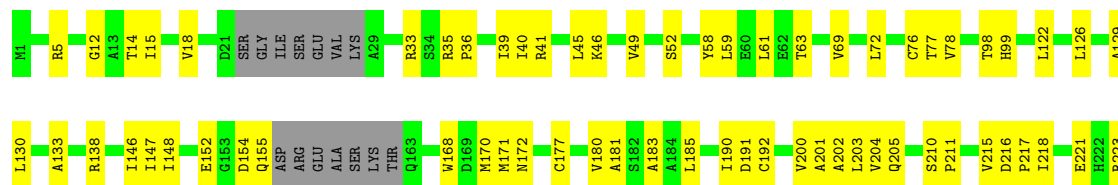
- Molecule 4: Exoribonuclease phosphorolytic domain-containing protein

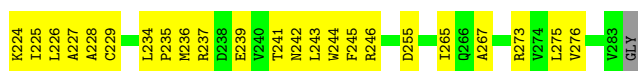


- Molecule 5: Exoribonuclease phosphorolytic domain-containing protein



- Molecule 6: Exosome complex component MTR3

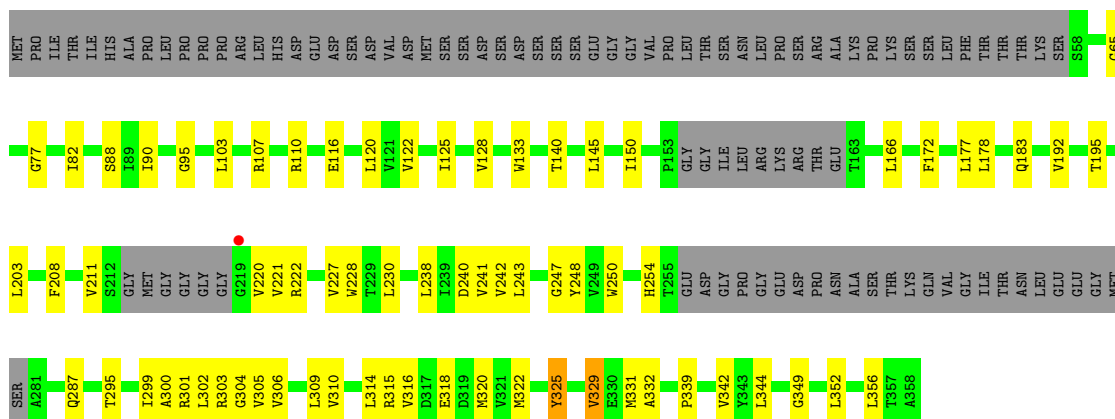




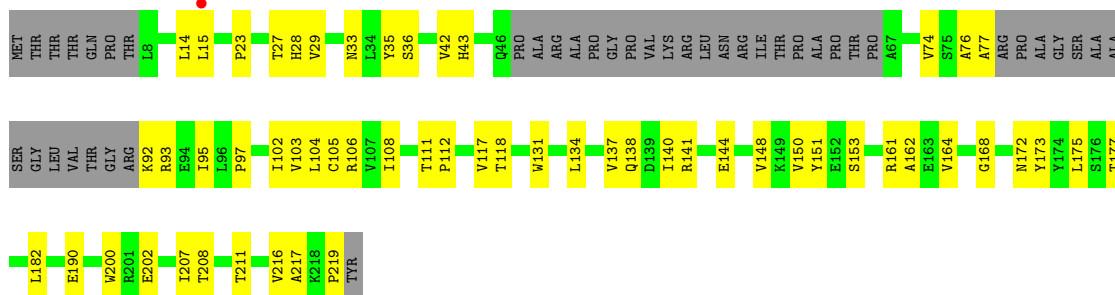
• Molecule 7: Ribosomal RNA-processing protein 40



• Molecule 8: Putative exosome complex protein



• Molecule 9: Putative exosome 3'->5' protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.53Å 148.38Å 195.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 3.81 48.90 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.90-3.81) 99.6 (48.90-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.243 , 0.292 0.243 , 0.293	Depositor DCC
R_{free} test set	1458 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	102.7	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	35554	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/2223	0.33	0/3021
2	B	0.17	0/1612	0.31	0/2182
3	C	0.18	0/2502	0.36	0/3399
4	D	0.15	0/1810	0.32	0/2462
5	E	0.27	0/2383	0.50	2/3253 (0.1%)
6	F	0.18	0/2063	0.39	0/2804
7	G	0.20	0/1966	0.41	0/2673
8	H	0.29	0/2021	0.51	2/2734 (0.1%)
9	I	0.22	0/1400	0.43	0/1906
All	All	0.21	0/17980	0.40	4/24434 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	H	329	VAL	N-CA-C	-6.25	104.25	110.62
5	E	208	ASP	N-CA-C	-5.77	102.96	109.60
5	E	209	PRO	N-CA-C	5.53	120.92	111.68
8	H	325	TYR	N-CA-C	-5.44	104.58	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2181	2195	2195	58	0
2	B	1594	1610	1606	45	0
3	C	2449	2490	2486	73	0
4	D	1775	1765	1764	47	0
5	E	2333	2393	2391	86	0
6	F	2028	2040	2038	86	0
7	G	1926	1971	1970	76	0
8	H	1993	2020	2016	50	0
9	I	1377	1414	1412	47	0
All	All	17656	17898	17878	529	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 15.

All (529) 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)
6:F:185:LEU:HD22	6:F:190:ILE:HG21	1.49	0.95
2:B:28:ALA:HB3	2:B:258:VAL:HG21	1.53	0.91
7:G:14:THR:HG22	7:G:43:ILE:HG12	1.59	0.84
9:I:14:LEU:HD11	9:I:33:ASN:HB3	1.60	0.84
3:C:274:VAL:HG12	3:C:293:ILE:HD13	1.57	0.84
1:A:233:ILE:HD11	2:B:234:VAL:HG22	1.58	0.83
7:G:125:ALA:HA	7:G:151:LEU:HD11	1.61	0.82
9:I:108:ILE:HD11	9:I:118:THR:HG23	1.60	0.81
3:C:89:LEU:HD21	3:C:94:ILE:HD13	1.66	0.77
9:I:97:PRO:HD2	9:I:131:TRP:CZ3	2.19	0.76
1:A:158:LEU:O	1:A:186:LEU:HD22	1.86	0.75
7:G:185:LEU:HD21	7:G:231:LEU:HD21	1.69	0.75
3:C:130:THR:HG23	6:F:147:ILE:HG21	1.69	0.74
2:B:164:LEU:HD22	2:B:255:LEU:HD23	1.70	0.73
6:F:49:VAL:HG21	6:F:58:TYR:HB2	1.69	0.73
8:H:82:ILE:HG23	8:H:88:SER:O	1.89	0.73
6:F:227:ALA:HB1	6:F:245:PHE:CE1	2.24	0.73
3:C:273:ALA:HB2	3:C:308:VAL:HG12	1.71	0.73
7:G:141:VAL:HG12	7:G:148:ALA:HB2	1.71	0.72
9:I:108:ILE:HD11	9:I:118:THR:CG2	2.18	0.72
5:E:203:SER:OG	5:E:210:TYR:N	2.22	0.72
7:G:15:ILE:HD11	7:G:42:ILE:HB	1.71	0.72
2:B:181:THR:O	2:B:201:LEU:HD23	1.90	0.72
9:I:23:PRO:HG3	9:I:29:VAL:HG21	1.72	0.71
8:H:211:VAL:HG22	8:H:247:GLY:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:42:VAL:HG22	9:I:74:VAL:HG22	1.73	0.71
8:H:302:LEU:O	8:H:305:VAL:HG22	1.90	0.71
2:B:23:LEU:HD21	2:B:44:MET:HE3	1.72	0.71
3:C:130:THR:CG2	6:F:147:ILE:HG21	2.22	0.70
4:D:149:THR:OG1	4:D:212:ILE:HD13	1.92	0.70
8:H:122:VAL:HG23	8:H:248:TYR:HB2	1.72	0.70
5:E:311:LEU:HD13	5:E:400:VAL:HG11	1.73	0.70
2:B:197:PRO:HB2	2:B:243:VAL:HG21	1.75	0.69
2:B:164:LEU:HD22	2:B:255:LEU:CD2	2.22	0.69
1:A:106:LEU:O	1:A:110:THR:HG23	1.92	0.69
7:G:163:VAL:HG13	7:G:235:ASP:OD2	1.92	0.69
5:E:187:LEU:HD12	5:E:407:LEU:HD11	1.75	0.68
5:E:10:LEU:C	5:E:11:LEU:HD12	2.17	0.68
6:F:49:VAL:HG21	6:F:58:TYR:CB	2.24	0.68
4:D:69:ARG:NE	4:D:118:SER:O	2.27	0.68
5:E:249:VAL:HG21	5:E:389:LEU:HD21	1.75	0.68
2:B:239:GLY:O	2:B:243:VAL:HG23	1.93	0.67
6:F:40:ILE:HD11	6:F:215:VAL:HG11	1.76	0.67
7:G:37:VAL:HG22	7:G:41:ASP:O	1.93	0.67
1:A:133:ILE:HD11	1:A:158:LEU:CD2	2.24	0.67
5:E:201:LEU:HD12	5:E:201:LEU:O	1.94	0.67
3:C:211:ILE:HD11	3:C:234:LEU:HD21	1.77	0.67
7:G:92:ILE:CD1	7:G:138:LEU:HD11	2.25	0.67
6:F:215:VAL:HG13	6:F:267:ALA:HB2	1.77	0.67
8:H:65:GLY:HA2	8:H:90:ILE:HD11	1.76	0.67
8:H:314:LEU:HD11	8:H:320:MET:HE1	1.77	0.66
5:E:272:LEU:HD12	5:E:389:LEU:HD22	1.75	0.66
5:E:45:GLU:CD	5:E:48:ILE:HD11	2.20	0.66
6:F:63:THR:OG1	6:F:69:VAL:HG12	1.96	0.66
6:F:203:LEU:HD23	6:F:226:LEU:HD13	1.76	0.66
7:G:208:VAL:HG13	7:G:214:VAL:HG22	1.76	0.66
7:G:140:CYS:O	7:G:151:LEU:HD12	1.94	0.66
3:C:66:HIS:O	3:C:85:ARG:NH1	2.29	0.66
7:G:216:VAL:HG21	7:G:227:VAL:HG11	1.78	0.65
9:I:137:VAL:HG12	9:I:150:VAL:HG22	1.77	0.65
5:E:37:THR:HG23	5:E:399:VAL:HG22	1.78	0.65
3:C:80:VAL:HG22	3:C:215:PHE:CE1	2.32	0.65
9:I:102:ILE:HD11	9:I:161:ARG:HG3	1.79	0.65
1:A:12:ARG:HG3	1:A:218:VAL:HG22	1.79	0.65
3:C:170:ILE:HD11	3:C:207:TRP:CD1	2.33	0.64
6:F:203:LEU:CD2	6:F:226:LEU:HD13	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:ILE:HG22	6:F:215:VAL:HB	1.80	0.64
6:F:78:VAL:HG23	6:F:146:ILE:CD1	2.28	0.64
9:I:137:VAL:HG12	9:I:150:VAL:CG2	2.27	0.64
7:G:14:THR:HG22	7:G:43:ILE:CG1	2.28	0.64
2:B:31:ARG:NH1	2:B:266:MET:SD	2.70	0.64
9:I:164:VAL:HG22	9:I:175:LEU:CD2	2.28	0.64
4:D:37:VAL:HG21	4:D:135:LEU:HD13	1.80	0.63
6:F:171:MET:HE1	6:F:228:ALA:C	2.23	0.63
1:A:83:LEU:HD23	1:A:91:PHE:CE1	2.33	0.63
8:H:145:LEU:HD21	8:H:150:ILE:HD11	1.81	0.63
6:F:122:LEU:HD21	6:F:170:MET:HG3	1.81	0.62
7:G:66:GLN:OE1	7:G:66:GLN:N	2.32	0.62
6:F:78:VAL:HG23	6:F:146:ILE:HD13	1.82	0.62
7:G:141:VAL:HG12	7:G:148:ALA:CB	2.30	0.62
8:H:203:LEU:HD13	8:H:250:TRP:CG	2.35	0.61
5:E:272:LEU:HD11	5:E:386:LEU:HD22	1.81	0.61
1:A:19:LEU:HD23	1:A:30:LEU:HD21	1.82	0.61
7:G:107:GLU:HB2	7:G:141:VAL:HG11	1.83	0.61
5:E:248:LEU:HD12	5:E:272:LEU:O	2.01	0.61
9:I:102:ILE:HD11	9:I:161:ARG:CG	2.31	0.61
1:A:15:VAL:HG11	1:A:218:VAL:HG21	1.82	0.60
6:F:41:ARG:HD2	6:F:218:ILE:HD11	1.83	0.60
7:G:101:LEU:HD21	7:G:106:PHE:CZ	2.36	0.60
1:A:87:THR:OG1	1:A:139:VAL:HG23	2.01	0.60
8:H:295:THR:HG22	8:H:299:ILE:HD11	1.83	0.60
4:D:84:ILE:HG23	4:D:144:ALA:O	2.02	0.60
9:I:14:LEU:CD1	9:I:33:ASN:HB3	2.31	0.60
2:B:163:THR:HG21	2:B:177:VAL:O	2.02	0.60
6:F:185:LEU:HD22	6:F:190:ILE:CG2	2.30	0.60
5:E:23:LEU:HD23	5:E:252:VAL:HG21	1.84	0.59
5:E:249:VAL:HG23	5:E:389:LEU:HD11	1.83	0.59
6:F:227:ALA:HB1	6:F:245:PHE:HE1	1.66	0.59
3:C:272:ALA:HB2	3:C:295:LEU:HD12	1.84	0.59
8:H:230:LEU:HD23	8:H:322:MET:SD	2.42	0.59
5:E:9:VAL:HG11	5:E:262:LYS:HD2	1.83	0.59
9:I:14:LEU:HD13	9:I:35:TYR:CE1	2.36	0.59
9:I:111:THR:HG23	9:I:112:PRO:HD2	1.85	0.59
1:A:79:ILE:HG23	1:A:135:VAL:HG13	1.83	0.59
3:C:121:LEU:HD23	3:C:168:LEU:HD12	1.85	0.59
7:G:141:VAL:HG12	7:G:148:ALA:CA	2.31	0.59
3:C:18:ILE:HD12	3:C:18:ILE:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:185:LEU:O	5:E:189:THR:HG23	2.03	0.59
9:I:141:ARG:HB3	9:I:148:VAL:HG21	1.84	0.59
7:G:46:VAL:HG21	7:G:63:TYR:CD1	2.38	0.59
2:B:51:CYS:HB2	2:B:145:LEU:CD2	2.33	0.59
6:F:133:ALA:HB1	6:F:192:CYS:SG	2.43	0.59
2:B:197:PRO:CB	2:B:243:VAL:HG21	2.33	0.58
3:C:329:GLY:O	4:D:83:GLN:NE2	2.36	0.58
1:A:158:LEU:C	1:A:186:LEU:HD22	2.28	0.58
5:E:149:ALA:HB2	6:F:246:ARG:HE	1.67	0.58
1:A:24:ARG:HD2	1:A:30:LEU:HD23	1.85	0.58
6:F:35:ARG:O	6:F:39:ILE:HB	2.04	0.58
6:F:41:ARG:HB2	6:F:61:LEU:HD11	1.86	0.58
7:G:81:LEU:HD11	7:G:91:LEU:HD11	1.84	0.58
3:C:49:ARG:NH2	3:C:295:LEU:O	2.37	0.58
3:C:59:VAL:HG22	3:C:73:VAL:HG22	1.85	0.58
4:D:84:ILE:HG21	4:D:132:MET:HE1	1.85	0.57
8:H:331:MET:HE1	8:H:352:LEU:HA	1.84	0.57
4:D:39:GLY:O	4:D:41:ILE:HG13	2.03	0.57
8:H:77:GLY:HA3	8:H:103:LEU:HD21	1.86	0.57
9:I:97:PRO:HD2	9:I:131:TRP:CE3	2.39	0.57
1:A:81:THR:HG22	1:A:104:SER:HB3	1.87	0.56
2:B:31:ARG:NH2	8:H:110:ARG:CZ	2.69	0.56
4:D:62:ALA:HB2	4:D:101:VAL:HG23	1.88	0.56
5:E:170:ASP:CG	5:E:172:LEU:HD21	2.30	0.56
5:E:120:VAL:HG22	5:E:148:LEU:HD21	1.87	0.56
7:G:46:VAL:HG21	7:G:63:TYR:CE1	2.40	0.56
7:G:167:PHE:CG	7:G:235:ASP:OD1	2.59	0.56
8:H:195:THR:HG22	8:H:195:THR:O	2.05	0.56
8:H:295:THR:HG22	8:H:299:ILE:CD1	2.36	0.56
5:E:280:ASP:OD1	5:E:309:ARG:NH2	2.38	0.56
1:A:26:ASP:OD2	1:A:32:GLN:NE2	2.38	0.56
1:A:133:ILE:HD11	1:A:158:LEU:HD22	1.88	0.56
5:E:65:GLU:O	5:E:173:LEU:HD12	2.06	0.56
7:G:208:VAL:HG13	7:G:214:VAL:CG2	2.36	0.56
6:F:243:LEU:HD23	6:F:243:LEU:C	2.31	0.56
2:B:147:VAL:HG21	2:B:154:LEU:HD11	1.86	0.55
1:A:195:VAL:HG21	1:A:256:ALA:HB1	1.86	0.55
3:C:162:LEU:HG	3:C:263:ILE:HG23	1.88	0.55
7:G:140:CYS:HA	7:G:151:LEU:HD12	1.88	0.55
1:A:245:GLU:HA	2:B:222:LYS:HA	1.87	0.55
3:C:268:ILE:HG21	3:C:352:VAL:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:LEU:HD23	2:B:24:ARG:N	2.22	0.55
2:B:21:ASN:HA	2:B:199:LEU:HD12	1.87	0.55
9:I:105:CYS:HB2	9:I:117:VAL:HG12	1.89	0.55
1:A:236:ILE:HD13	2:B:228:CYS:HB3	1.88	0.55
5:E:49:LEU:HD23	5:E:50:PRO:O	2.07	0.54
7:G:92:ILE:HD11	7:G:138:LEU:HD11	1.89	0.54
1:A:144:GLY:HA2	1:A:211:ALA:O	2.06	0.54
1:A:66:VAL:HG21	6:F:12:GLY:CA	2.37	0.54
6:F:59:LEU:HB2	6:F:180:VAL:HG12	1.89	0.54
9:I:108:ILE:CD1	9:I:118:THR:HG23	2.35	0.54
9:I:106:ARG:C	9:I:117:VAL:HG13	2.32	0.54
8:H:300:ALA:HB3	8:H:342:VAL:HG11	1.88	0.54
5:E:212:ASP:OD1	5:E:213:ASP:N	2.40	0.54
7:G:240:THR:O	7:G:243:GLY:N	2.41	0.54
7:G:248:VAL:O	7:G:252:LEU:HD13	2.08	0.54
7:G:184:VAL:HG22	7:G:187:MET:CE	2.38	0.54
2:B:236:ARG:HB3	2:B:240:MET:HE2	1.90	0.54
5:E:9:VAL:HG11	5:E:262:LYS:CD	2.38	0.53
5:E:383:ARG:HD2	6:F:265:ILE:HD13	1.89	0.53
3:C:82:CYS:SG	3:C:213:LEU:HD11	2.48	0.53
5:E:122:ILE:HG12	5:E:169:ILE:CG2	2.39	0.53
5:E:313:LEU:HD11	5:E:316:ILE:HG13	1.91	0.53
1:A:24:ARG:NH2	1:A:210:ASP:O	2.42	0.53
1:A:66:VAL:HG21	6:F:12:GLY:HA2	1.89	0.53
9:I:162:ALA:HA	9:I:182:LEU:HD13	1.91	0.53
3:C:121:LEU:HD11	3:C:206:TYR:HB3	1.91	0.53
3:C:130:THR:CB	3:C:138:PRO:HB3	2.39	0.52
9:I:140:ILE:HG21	9:I:153:SER:HB3	1.91	0.52
1:A:144:GLY:CA	1:A:211:ALA:O	2.57	0.52
4:D:57:VAL:C	4:D:58:ILE:HD13	2.34	0.52
6:F:202:ALA:CB	6:F:225:ILE:HD11	2.39	0.52
7:G:45:THR:O	7:G:45:THR:HG22	2.10	0.52
6:F:215:VAL:CG1	6:F:267:ALA:HB2	2.40	0.52
7:G:184:VAL:HG22	7:G:187:MET:HE3	1.92	0.52
3:C:313:VAL:HG13	3:C:321:ARG:O	2.09	0.52
6:F:218:ILE:HG21	6:F:221:GLU:OE1	2.10	0.52
7:G:89:LEU:HD23	7:G:99:ALA:O	2.09	0.52
2:B:31:ARG:HH22	8:H:110:ARG:CZ	2.23	0.51
2:B:237:LEU:HA	2:B:240:MET:HE3	1.93	0.51
5:E:381:ALA:O	6:F:239:GLU:HA	2.10	0.51
9:I:137:VAL:HA	9:I:140:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PHE:CD2	1:A:244:VAL:HG21	2.45	0.51
8:H:120:LEU:C	8:H:120:LEU:HD23	2.34	0.51
1:A:103:LEU:HD13	1:A:147:VAL:HG22	1.91	0.51
1:A:165:ASP:OD1	1:A:166:THR:N	2.44	0.51
3:C:311:MET:HE2	3:C:325:ILE:HG12	1.91	0.51
3:C:130:THR:HB	3:C:138:PRO:HB3	1.93	0.51
2:B:241:LEU:O	2:B:245:VAL:HG23	2.11	0.51
5:E:122:ILE:HG12	5:E:169:ILE:HG21	1.93	0.51
8:H:150:ILE:HD12	8:H:172:PHE:CE1	2.46	0.51
2:B:212:LEU:C	2:B:212:LEU:HD23	2.36	0.51
3:C:130:THR:OG1	3:C:138:PRO:CD	2.59	0.51
3:C:210:TYR:OH	6:F:14:THR:HG21	2.11	0.51
6:F:130:LEU:HD21	6:F:181:ALA:HB3	1.92	0.51
8:H:211:VAL:HG21	8:H:220:VAL:HG13	1.93	0.51
8:H:221:VAL:HG22	8:H:316:VAL:O	2.10	0.51
3:C:131:GLY:HA2	6:F:77:THR:HG21	1.93	0.50
3:C:170:ILE:HD11	3:C:207:TRP:NE1	2.26	0.50
3:C:327:LYS:O	4:D:190:LEU:HD12	2.10	0.50
7:G:167:PHE:CD2	7:G:235:ASP:OD1	2.64	0.50
2:B:166:CYS:HB3	2:B:171:ILE:HD11	1.92	0.50
9:I:202:GLU:HB3	9:I:211:THR:HG22	1.94	0.50
1:A:233:ILE:O	2:B:231:ARG:HA	2.10	0.50
5:E:256:ILE:HD13	5:E:389:LEU:HA	1.92	0.50
8:H:230:LEU:HG	8:H:322:MET:HE1	1.94	0.50
3:C:80:VAL:HG22	3:C:215:PHE:CD1	2.46	0.50
7:G:37:VAL:CG2	7:G:41:ASP:HB3	2.41	0.50
7:G:171:LEU:HD11	7:G:182:VAL:HG11	1.93	0.50
3:C:45:ARG:NH1	3:C:301:GLU:OE1	2.43	0.50
7:G:172:LEU:CD2	7:G:210:ARG:HG2	2.42	0.50
1:A:139:VAL:HG23	1:A:139:VAL:O	2.12	0.50
4:D:33:VAL:HG22	4:D:101:VAL:HG12	1.94	0.50
8:H:227:VAL:HG22	8:H:242:VAL:HG22	1.94	0.50
4:D:107:ASN:CG	4:D:110:VAL:HG22	2.37	0.50
7:G:172:LEU:HD12	7:G:208:VAL:HB	1.94	0.49
1:A:20:GLN:HA	1:A:206:ILE:HD11	1.93	0.49
1:A:116:ALA:HB2	1:A:190:HIS:O	2.12	0.49
7:G:192:ASP:OD1	7:G:194:SER:N	2.45	0.49
3:C:121:LEU:HD12	3:C:208:VAL:HG22	1.93	0.49
7:G:6:ARG:N	7:G:7:PRO:CD	2.75	0.49
2:B:23:LEU:HD23	2:B:24:ARG:H	1.75	0.49
6:F:202:ALA:HB1	6:F:225:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:VAL:HG12	7:G:148:ALA:HA	1.94	0.49
1:A:155:VAL:HG11	1:A:192:PRO:O	2.13	0.49
3:C:64:LEU:HD21	3:C:81:LEU:HD21	1.95	0.49
7:G:36:HIS:ND1	7:G:37:VAL:O	2.43	0.49
8:H:306:VAL:O	8:H:310:VAL:HG13	2.12	0.49
6:F:235:PRO:O	6:F:236:MET:HB2	2.12	0.49
8:H:309:LEU:HD21	8:H:356:LEU:CD1	2.42	0.49
9:I:144:GLU:O	9:I:148:VAL:HG23	2.13	0.49
3:C:156:LEU:HD23	3:C:227:TRP:CD2	2.48	0.48
5:E:119:TRP:CD1	5:E:164:HIS:CE1	3.01	0.48
5:E:276:VAL:HG21	5:E:400:VAL:HG21	1.94	0.48
8:H:128:VAL:HG22	8:H:133:TRP:CZ3	2.48	0.48
5:E:315:SER:HA	6:F:245:PHE:O	2.13	0.48
5:E:316:ILE:O	6:F:244:TRP:HA	2.12	0.48
6:F:147:ILE:C	6:F:148:ILE:HD13	2.39	0.48
5:E:194:LEU:C	5:E:194:LEU:HD23	2.39	0.48
4:D:27:SER:HA	4:D:31:TYR:O	2.14	0.48
6:F:172:ASN:OD1	6:F:217:PRO:HG3	2.14	0.48
7:G:102:PRO:HB2	7:G:105:ALA:HB2	1.96	0.48
3:C:130:THR:OG1	3:C:138:PRO:HD3	2.14	0.48
3:C:167:GLU:HG3	3:C:261:LEU:HD11	1.96	0.48
5:E:139:LEU:HD11	5:E:180:TYR:OH	2.13	0.48
9:I:104:LEU:N	9:I:104:LEU:HD22	2.29	0.48
3:C:121:LEU:HD11	3:C:206:TYR:CB	2.44	0.48
7:G:148:ALA:HB1	7:G:151:LEU:O	2.13	0.48
4:D:107:ASN:OD1	4:D:110:VAL:HG22	2.14	0.47
2:B:53:VAL:HG13	2:B:143:ILE:HD13	1.96	0.47
3:C:72:LEU:HD11	3:C:79:THR:CG2	2.44	0.47
6:F:171:MET:HE1	6:F:229:CYS:N	2.29	0.47
7:G:185:LEU:CD2	7:G:231:LEU:HD21	2.40	0.47
4:D:120:ASN:ND2	4:D:123:VAL:HG23	2.30	0.47
5:E:171:ILE:C	5:E:172:LEU:HD23	2.39	0.47
4:D:141:PRO:HA	7:G:45:THR:HG22	1.95	0.47
6:F:59:LEU:HD23	6:F:59:LEU:C	2.40	0.47
1:A:142:HIS:CD2	1:A:213:TRP:CZ3	3.02	0.47
3:C:293:ILE:C	3:C:294:LEU:HD12	2.39	0.47
1:A:142:HIS:ND1	1:A:146:LEU:CD2	2.77	0.47
5:E:194:LEU:HD22	5:E:412:LEU:CD1	2.44	0.47
6:F:202:ALA:HA	6:F:228:ALA:HA	1.96	0.47
2:B:26:VAL:HG11	2:B:254:ILE:HD12	1.97	0.47
6:F:36:PRO:HA	6:F:39:ILE:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:LEU:HD23	3:C:168:LEU:CD1	2.45	0.47
6:F:76:CYS:HB2	6:F:148:ILE:HD12	1.97	0.46
7:G:53:ASN:O	7:G:56:LYS:O	2.33	0.46
3:C:148:THR:HG22	4:D:72:HIS:HA	1.96	0.46
5:E:166:LYS:HG2	5:E:168:TYR:CE1	2.51	0.46
3:C:78:THR:OG1	3:C:220:GLY:N	2.49	0.46
6:F:39:ILE:HG21	6:F:216:ASP:H	1.81	0.46
4:D:25:ARG:HG3	4:D:34:THR:CG2	2.46	0.46
5:E:222:PHE:HB3	5:E:243:PRO:HD3	1.97	0.46
6:F:204:VAL:HG22	6:F:205:GLN:N	2.30	0.46
7:G:29:ARG:O	7:G:58:SER:HA	2.14	0.46
9:I:15:LEU:HD11	9:I:36:SER:HB2	1.97	0.46
5:E:39:PHE:CE2	5:E:403:VAL:HG21	2.51	0.46
1:A:51:PHE:O	1:A:54:THR:HG22	2.15	0.46
1:A:124:LEU:HD12	1:A:130:CYS:HA	1.97	0.46
1:A:243:PRO:HG3	2:B:217:LEU:HD22	1.97	0.46
6:F:154:ASP:O	6:F:155:GLN:HB3	2.15	0.46
7:G:133:HIS:NE2	9:I:190:GLU:OE1	2.49	0.46
3:C:126:ILE:HD12	3:C:213:LEU:HD22	1.96	0.46
5:E:309:ARG:O	5:E:396:LYS:CD	2.64	0.46
5:E:122:ILE:HA	5:E:169:ILE:HG23	1.98	0.46
7:G:163:VAL:HA	7:G:235:ASP:OD2	2.16	0.46
4:D:81:PHE:CZ	4:D:131:ALA:HB3	2.51	0.46
9:I:161:ARG:O	9:I:182:LEU:HB3	2.15	0.46
1:A:79:ILE:HG23	1:A:135:VAL:CG1	2.46	0.46
2:B:56:PRO:O	8:H:140:THR:HA	2.16	0.45
4:D:120:ASN:HD21	4:D:123:VAL:HG23	1.80	0.45
5:E:201:LEU:HB3	5:E:211:PHE:CE1	2.51	0.45
5:E:389:LEU:C	5:E:389:LEU:HD23	2.40	0.45
6:F:126:LEU:HD11	6:F:130:LEU:HD11	1.99	0.45
6:F:130:LEU:HD11	6:F:181:ALA:HB1	1.97	0.45
9:I:168:GLY:HA2	9:I:173:TYR:HA	1.97	0.45
4:D:168:PRO:O	4:D:171:VAL:HG22	2.16	0.45
7:G:202:LEU:HD11	7:G:223:THR:OG1	2.15	0.45
3:C:212:ASP:C	3:C:213:LEU:HD12	2.41	0.45
4:D:41:ILE:HG22	4:D:42:GLU:O	2.16	0.45
8:H:195:THR:O	8:H:195:THR:CG2	2.65	0.45
1:A:28:ARG:HB3	1:A:32:GLN:HG2	1.99	0.45
5:E:58:VAL:HB	5:E:184:LEU:HD11	1.97	0.45
7:G:171:LEU:CD1	7:G:182:VAL:HG11	2.46	0.45
7:G:223:THR:O	7:G:227:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:332:ALA:HB1	8:H:339:PRO:HA	1.99	0.45
7:G:184:VAL:HG23	7:G:244:GLN:OE1	2.16	0.45
9:I:217:ALA:HB1	9:I:219:PRO:HD2	1.98	0.45
3:C:164:SER:N	3:C:167:GLU:OE2	2.50	0.45
7:G:163:VAL:HG13	7:G:235:ASP:CG	2.41	0.45
1:A:79:ILE:HD12	1:A:108:GLU:HA	1.99	0.45
4:D:94:LEU:HD23	4:D:94:LEU:C	2.41	0.45
5:E:30:ARG:HD3	5:E:34:ARG:O	2.16	0.45
5:E:70:VAL:CG1	5:E:167:LEU:HG	2.47	0.45
5:E:371:GLU:CG	5:E:372:GLY:N	2.80	0.45
1:A:204:GLY:HA3	1:A:244:VAL:HG22	1.99	0.45
5:E:14:ALA:O	5:E:17:ALA:N	2.50	0.45
5:E:46:THR:CG2	5:E:195:SER:HB2	2.47	0.45
7:G:78:ALA:HB3	7:G:123:VAL:HG23	1.99	0.45
3:C:25:HIS:HB3	3:C:26:PRO:HD3	1.98	0.45
6:F:223:ARG:HG3	6:F:224:LYS:N	2.32	0.45
8:H:103:LEU:HD23	8:H:103:LEU:C	2.42	0.45
4:D:159:ALA:O	4:D:160:THR:HG23	2.16	0.45
5:E:363:ILE:HG23	5:E:363:ILE:O	2.17	0.45
3:C:55:ARG:HB2	3:C:296:ASP:OD2	2.17	0.44
5:E:407:LEU:HA	5:E:410:VAL:HG23	2.00	0.44
9:I:33:ASN:O	9:I:35:TYR:CE2	2.70	0.44
1:A:151:CYS:O	1:A:155:VAL:HG13	2.17	0.44
2:B:179:ALA:HB2	2:B:215:ALA:HB2	1.99	0.44
3:C:140:VAL:HG12	3:C:141:PRO:HD2	1.99	0.44
3:C:309:ILE:HA	3:C:326:GLU:O	2.17	0.44
5:E:242:ARG:NH1	5:E:404:LEU:HG	2.32	0.44
6:F:183:ALA:HB2	6:F:275:LEU:HD13	1.99	0.44
7:G:15:ILE:HD12	7:G:20:VAL:CG2	2.46	0.44
8:H:116:GLU:OE1	8:H:222:ARG:NH1	2.50	0.44
1:A:266:LEU:HD23	1:A:266:LEU:C	2.42	0.44
2:B:31:ARG:HH22	8:H:110:ARG:NH2	2.15	0.44
5:E:142:LEU:O	5:E:142:LEU:HD23	2.17	0.44
5:E:186:SER:CB	5:E:246:THR:O	2.65	0.44
5:E:272:LEU:HD11	5:E:386:LEU:CD2	2.47	0.44
5:E:126:ILE:HG23	5:E:127:PRO:HD2	2.00	0.44
1:A:43:GLN:NE2	4:D:104:SER:O	2.50	0.44
3:C:163:VAL:HG11	3:C:234:LEU:HD22	2.00	0.44
4:D:91:PRO:HG3	7:G:132:ARG:O	2.17	0.44
4:D:167:SER:HB2	4:D:168:PRO:HD2	2.00	0.44
7:G:230:ALA:HB2	7:G:251:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:303:ARG:O	8:H:306:VAL:HG12	2.17	0.44
7:G:107:GLU:CB	7:G:141:VAL:HG11	2.46	0.44
8:H:241:VAL:HG22	8:H:243:LEU:CD2	2.48	0.44
3:C:340:SER:OG	3:C:343:LEU:HD12	2.16	0.44
5:E:242:ARG:HG2	5:E:280:ASP:OD1	2.18	0.44
6:F:218:ILE:HG22	6:F:218:ILE:O	2.17	0.44
2:B:166:CYS:SG	2:B:171:ILE:HD11	2.58	0.43
3:C:19:PHE:O	3:C:22:LEU:O	2.35	0.43
3:C:274:VAL:CG2	3:C:307:GLU:HB3	2.47	0.43
4:D:213:CYS:O	4:D:239:ARG:HG3	2.18	0.43
6:F:255:ASP:N	6:F:255:ASP:OD1	2.51	0.43
7:G:37:VAL:HG21	7:G:41:ASP:HB3	1.99	0.43
8:H:240:ASP:OD2	8:H:254:HIS:HA	2.19	0.43
3:C:126:ILE:CD1	3:C:213:LEU:HD22	2.48	0.43
7:G:216:VAL:HG21	7:G:227:VAL:CG1	2.46	0.43
9:I:92:LYS:HE3	9:I:92:LYS:HA	1.99	0.43
2:B:51:CYS:CB	2:B:145:LEU:CD2	2.96	0.43
3:C:93:ARG:HH21	6:F:15:ILE:HD11	1.83	0.43
5:E:23:LEU:CD2	5:E:252:VAL:HG21	2.47	0.43
7:G:122:LEU:HD11	7:G:160:VAL:HG11	1.99	0.43
6:F:130:LEU:HD11	6:F:181:ALA:CB	2.48	0.43
6:F:210:SER:N	6:F:211:PRO:CD	2.81	0.43
6:F:237:ARG:NH1	6:F:239:GLU:OE1	2.51	0.43
7:G:131:ASN:ND2	9:I:151:TYR:OH	2.51	0.43
7:G:172:LEU:HD22	7:G:210:ARG:HG2	1.99	0.43
3:C:134:PRO:HD3	6:F:52:SER:HB2	2.00	0.43
3:C:170:ILE:O	3:C:203:VAL:HG13	2.18	0.43
3:C:348:ARG:O	3:C:351:VAL:HG22	2.18	0.43
4:D:25:ARG:HG3	4:D:34:THR:HG22	2.00	0.43
5:E:249:VAL:HG21	5:E:389:LEU:CD2	2.46	0.43
5:E:323:SER:O	5:E:326:THR:OG1	2.36	0.43
7:G:75:LEU:HD11	7:G:126:ARG:NH1	2.33	0.43
8:H:238:LEU:N	8:H:238:LEU:HD12	2.33	0.43
1:A:81:THR:OG1	1:A:103:LEU:HD23	2.19	0.43
1:A:250:LEU:HD21	2:B:238:GLU:HB3	2.00	0.43
5:E:42:LEU:HD21	5:E:58:VAL:HG11	2.01	0.43
5:E:324:ARG:HA	5:E:376:ALA:HB1	2.00	0.43
5:E:383:ARG:CD	6:F:265:ILE:HD13	2.48	0.43
5:E:413:THR:HG23	5:E:413:THR:O	2.18	0.43
6:F:45:LEU:HD23	6:F:46:LYS:N	2.34	0.43
6:F:234:LEU:HD12	6:F:234:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:CYS:CB	2:B:171:ILE:HD11	2.49	0.43
3:C:31:THR:HB	3:C:44:GLN:O	2.19	0.43
6:F:138:ARG:NH2	9:I:27:THR:O	2.51	0.43
7:G:51:ILE:HG22	7:G:60:TRP:O	2.19	0.43
7:G:215:TRP:CH2	7:G:217:GLY:HA3	2.54	0.43
8:H:301:ARG:HB2	8:H:342:VAL:HG13	2.00	0.43
1:A:117:LEU:HD21	1:A:188:TRP:CZ3	2.54	0.43
1:A:202:ASP:O	1:A:203:GLU:HB2	2.19	0.43
5:E:120:VAL:CG2	5:E:148:LEU:HD21	2.48	0.43
5:E:122:ILE:HA	5:E:169:ILE:CG2	2.49	0.43
8:H:331:MET:CE	8:H:352:LEU:HA	2.48	0.43
3:C:215:PHE:CD1	3:C:215:PHE:N	2.87	0.42
5:E:240:THR:OG1	5:E:280:ASP:HB2	2.19	0.42
5:E:309:ARG:O	5:E:396:LYS:HD2	2.18	0.42
6:F:78:VAL:HG21	6:F:185:LEU:HD23	2.01	0.42
7:G:67:ARG:C	7:G:165:LEU:HD11	2.44	0.42
8:H:95:GLY:HA3	8:H:107:ARG:O	2.18	0.42
8:H:221:VAL:HG11	8:H:315:ARG:HB2	2.01	0.42
8:H:325:TYR:O	8:H:329:VAL:HG23	2.18	0.42
1:A:1:MET:HE3	1:A:90:THR:HA	2.02	0.42
6:F:205:GLN:HA	6:F:210:SER:HA	2.01	0.42
7:G:45:THR:O	7:G:45:THR:CG2	2.67	0.42
7:G:249:ARG:HG2	7:G:250:ARG:N	2.32	0.42
8:H:128:VAL:HG22	8:H:133:TRP:HZ3	1.83	0.42
8:H:178:LEU:HD12	8:H:178:LEU:C	2.44	0.42
3:C:338:ILE:HD13	4:D:202:TRP:CH2	2.53	0.42
5:E:197:ARG:HD3	5:E:220:TYR:CE1	2.55	0.42
6:F:129:ALA:HA	6:F:241:THR:CG2	2.50	0.42
1:A:1:MET:HG3	4:D:42:GLU:HG3	2.00	0.42
4:D:145:THR:O	4:D:184:SER:N	2.53	0.42
6:F:72:LEU:CD1	6:F:152:GLU:O	2.67	0.42
9:I:111:THR:HG23	9:I:112:PRO:CD	2.47	0.42
9:I:162:ALA:HB2	9:I:177:THR:HG22	2.00	0.42
4:D:183:THR:HG22	4:D:184:SER:N	2.33	0.42
4:D:209:ALA:O	4:D:212:ILE:HG12	2.19	0.42
5:E:332:ASN:HB2	8:H:287:GLN:CD	2.45	0.42
6:F:72:LEU:HD12	6:F:152:GLU:O	2.19	0.42
6:F:200:VAL:HG12	6:F:201:ALA:N	2.35	0.42
6:F:234:LEU:O	6:F:237:ARG:O	2.37	0.42
1:A:54:THR:HB	1:A:143:ASP:H	1.83	0.42
3:C:22:LEU:O	3:C:23:SER:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:LEU:HD22	4:D:127:LEU:HD22	2.02	0.42
9:I:93:ARG:CG	9:I:95:ILE:HG13	2.50	0.42
2:B:20:TRP:CG	2:B:21:ASN:N	2.87	0.42
3:C:137:LEU:HB3	3:C:138:PRO:CD	2.50	0.42
3:C:215:PHE:N	3:C:215:PHE:HD1	2.18	0.42
5:E:262:LYS:HG3	5:E:263:GLU:N	2.34	0.42
6:F:39:ILE:CG2	6:F:215:VAL:HB	2.49	0.42
8:H:125:ILE:HD13	8:H:172:PHE:HB3	2.01	0.42
8:H:300:ALA:O	8:H:304:GLY:N	2.48	0.42
9:I:103:VAL:HG22	9:I:162:ALA:O	2.18	0.42
2:B:210:PRO:HB2	2:B:232:VAL:CG1	2.50	0.42
7:G:72:GLN:NE2	7:G:128:SER:O	2.51	0.42
9:I:102:ILE:HD11	9:I:161:ARG:HG2	2.01	0.42
1:A:103:LEU:HD11	1:A:107:LEU:HD11	2.01	0.42
2:B:199:LEU:HD22	2:B:247:GLY:CA	2.50	0.42
4:D:57:VAL:O	4:D:58:ILE:HD13	2.18	0.42
5:E:49:LEU:HB3	5:E:55:SER:CB	2.50	0.42
8:H:228:TRP:CH2	8:H:318:GLU:HA	2.54	0.42
1:A:163:LYS:HE2	1:A:186:LEU:HA	2.02	0.41
2:B:33:GLN:HG2	2:B:36:ALA:HB2	2.01	0.41
4:D:256:TRP:CG	7:G:170:ARG:NH1	2.88	0.41
5:E:126:ILE:HB	5:E:129:VAL:HB	2.02	0.41
6:F:18:VAL:HG23	6:F:18:VAL:O	2.20	0.41
6:F:171:MET:HG2	6:F:244:TRP:CE2	2.54	0.41
9:I:200:TRP:O	9:I:216:VAL:HG12	2.20	0.41
3:C:138:PRO:HB2	6:F:99:HIS:ND1	2.35	0.41
6:F:273:ARG:HA	6:F:276:VAL:HG22	2.02	0.41
3:C:278:LYS:HE2	3:C:278:LYS:HA	2.02	0.41
5:E:264:GLU:O	5:E:267:VAL:HG22	2.20	0.41
6:F:226:LEU:HD12	6:F:226:LEU:H	1.85	0.41
4:D:14:LEU:HD11	4:D:133:LEU:HB3	2.02	0.41
4:D:31:TYR:OH	4:D:122:ALA:HB1	2.20	0.41
9:I:134:LEU:HD13	9:I:172:ASN:HB3	2.02	0.41
1:A:87:THR:CG2	1:A:142:HIS:HB2	2.50	0.41
1:A:148:ASP:OD2	1:A:196:THR:HB	2.21	0.41
5:E:169:ILE:HD11	5:E:189:THR:HG22	2.02	0.41
9:I:28:HIS:O	9:I:28:HIS:CG	2.73	0.41
1:A:36:LEU:HB2	1:A:51:PHE:CE1	2.56	0.41
1:A:135:VAL:HG13	1:A:135:VAL:O	2.20	0.41
2:B:52:VAL:O	2:B:52:VAL:HG23	2.19	0.41
7:G:9:VAL:O	7:G:10:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:33:ASN:O	9:I:35:TYR:CD2	2.74	0.41
5:E:166:LYS:HE2	5:E:168:TYR:CE2	2.55	0.41
8:H:177:LEU:HD21	8:H:208:PHE:CD1	2.56	0.41
8:H:344:LEU:O	8:H:349:GLY:CA	2.68	0.41
9:I:42:VAL:HG12	9:I:43:HIS:N	2.35	0.41
9:I:207:ILE:HG13	9:I:208:THR:N	2.36	0.41
2:B:145:LEU:HD13	2:B:158:LEU:CD2	2.51	0.41
3:C:293:ILE:HD12	3:C:333:PHE:CZ	2.55	0.41
4:D:246:MET:O	4:D:250:VAL:HG23	2.21	0.41
5:E:14:ALA:O	5:E:17:ALA:HB3	2.21	0.41
5:E:221:LEU:HG	5:E:222:PHE:CD2	2.56	0.41
6:F:39:ILE:O	6:F:40:ILE:C	2.64	0.41
6:F:126:LEU:HD22	6:F:177:CYS:HB3	2.03	0.41
3:C:54:ALA:HB1	3:C:348:ARG:NH1	2.36	0.41
3:C:307:GLU:HA	3:C:328:GLN:O	2.21	0.41
4:D:69:ARG:HG2	4:D:70:GLU:N	2.36	0.41
4:D:211:ASN:O	4:D:215:ARG:HD3	2.20	0.41
5:E:187:LEU:HD12	5:E:407:LEU:CD1	2.47	0.41
5:E:400:VAL:HG13	5:E:401:ASP:N	2.35	0.41
7:G:106:PHE:O	7:G:109:ALA:HB2	2.21	0.41
3:C:47:ASN:ND2	3:C:301:GLU:OE2	2.54	0.41
3:C:116:LEU:HD21	3:C:165:ALA:HA	2.01	0.41
4:D:182:PHE:CZ	4:D:188:LEU:HD21	2.55	0.41
5:E:16:LEU:HD13	5:E:374:TRP:CZ3	2.56	0.41
5:E:129:VAL:HG12	5:E:130:ARG:O	2.20	0.41
6:F:33:ARG:NH1	6:F:39:ILE:O	2.52	0.41
6:F:168:TRP:CE2	6:F:225:ILE:CG2	3.04	0.41
6:F:191:ASP:OD1	6:F:191:ASP:N	2.54	0.41
7:G:16:ASP:HB2	7:G:19:LEU:HD12	2.02	0.41
7:G:240:THR:O	7:G:241:ILE:C	2.64	0.41
8:H:183:GLN:N	8:H:192:VAL:O	2.54	0.41
9:I:76:ALA:O	9:I:77:ALA:C	2.64	0.41
2:B:126:ALA:HB2	2:B:225:VAL:HG21	2.03	0.40
2:B:179:ALA:HB2	2:B:215:ALA:CB	2.51	0.40
4:D:124:MET:N	4:D:125:PRO:HD2	2.36	0.40
5:E:266:ALA:O	5:E:323:SER:HB3	2.21	0.40
6:F:98:THR:HG21	6:F:126:LEU:HG	2.03	0.40
7:G:77:LEU:HD21	7:G:160:VAL:HG12	2.02	0.40
7:G:231:LEU:HD23	7:G:231:LEU:HA	1.97	0.40
3:C:143:THR:HG23	3:C:146:ALA:H	1.86	0.40
5:E:159:ILE:O	5:E:160:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:313:LEU:HD12	5:E:314:LEU:N	2.36	0.40
1:A:161:PHE:HD2	1:A:186:LEU:HD13	1.87	0.40
2:B:51:CYS:CB	2:B:145:LEU:HD23	2.51	0.40
4:D:56:ASP:OD2	4:D:58:ILE:HD11	2.22	0.40
4:D:81:PHE:CE1	4:D:132:MET:HE2	2.57	0.40
9:I:137:VAL:HG23	9:I:138:GLN:N	2.37	0.40
3:C:211:ILE:CD1	3:C:234:LEU:HD21	2.49	0.40
1:A:117:LEU:HD13	1:A:133:ILE:HD13	2.03	0.40
3:C:142:PRO:HD2	6:F:5:ARG:HD2	2.03	0.40
4:D:73:LEU:CD1	4:D:124:MET:HE3	2.52	0.40
6:F:204:VAL:CG2	6:F:205:GLN:N	2.85	0.40
6:F:242:ASN:OD1	6:F:243:LEU:N	2.55	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	279/293 (95%)	272 (98%)	7 (2%)	0	100	100
2	B	203/284 (72%)	200 (98%)	3 (2%)	0	100	100
3	C	303/357 (85%)	295 (97%)	8 (3%)	0	100	100
4	D	228/258 (88%)	224 (98%)	4 (2%)	0	100	100
5	E	294/413 (71%)	287 (98%)	6 (2%)	1 (0%)	36	68
6	F	263/284 (93%)	252 (96%)	11 (4%)	0	100	100
7	G	249/256 (97%)	242 (97%)	7 (3%)	0	100	100
8	H	253/358 (71%)	250 (99%)	3 (1%)	0	100	100
9	I	172/220 (78%)	169 (98%)	3 (2%)	0	100	100
All	All	2244/2723 (82%)	2191 (98%)	52 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	181	PRO

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	243/253 (96%)	243 (100%)	0	100	100
2	B	175/222 (79%)	175 (100%)	0	100	100
3	C	269/303 (89%)	269 (100%)	0	100	100
4	D	189/211 (90%)	189 (100%)	0	100	100
5	E	257/339 (76%)	257 (100%)	0	100	100
6	F	223/235 (95%)	223 (100%)	0	100	100
7	G	212/217 (98%)	212 (100%)	0	100	100
8	H	212/293 (72%)	211 (100%)	1 (0%)	81	81
9	I	152/184 (83%)	152 (100%)	0	100	100
All	All	1932/2257 (86%)	1931 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	166	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	94	ASN
1	A	128	GLN
2	B	204	GLN
4	D	175	GLN
5	E	160	ASN

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Mol	Chain	Res	Type
5	E	332	ASN
6	F	38	ASN
7	G	85	GLN
8	H	141	GLN
8	H	351	GLN
9	I	101	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9	
1	A	281/293 (95%)	-0.18	0	100	100	85, 114, 143, 177	4 (1%)
2	B	211/284 (74%)	-0.25	0	100	100	84, 106, 135, 158	3 (1%)
3	C	311/357 (87%)	-0.07	0	100	100	81, 109, 144, 171	0
4	D	232/258 (89%)	-0.13	0	100	100	88, 106, 133, 149	0
5	E	304/413 (73%)	-0.06	0	100	100	81, 107, 132, 155	0
6	F	269/284 (94%)	-0.03	0	100	100	86, 108, 146, 156	1 (0%)
7	G	251/256 (98%)	-0.24	0	100	100	96, 117, 148, 167	0
8	H	261/358 (72%)	-0.14	1 (0%)	88	75	81, 107, 131, 152	0
9	I	178/220 (80%)	-0.09	1 (0%)	85	69	94, 128, 152, 160	0
All	All	2298/2723 (84%)	-0.13	2 (0%)	92	87	81, 111, 143, 177	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	219	GLY	2.3
9	I	15	LEU	2.2

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.