



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:31 AM EDT

PDB ID : 8W8N / pdb_00008w8n
Title : Thermus thermophilus initiation transcription complex in the pre-translocated state
Authors : Li, L.; Zhang, Y.
Deposited on : 2023-09-04
Resolution : 2.69 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

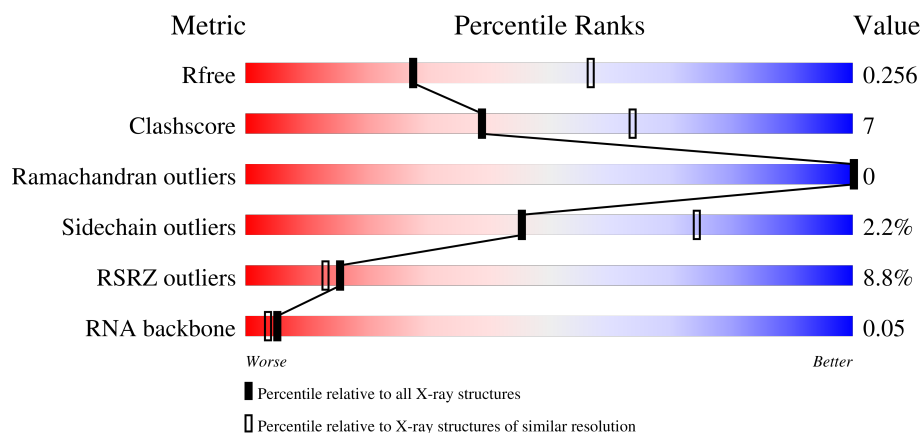
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	315	
1	B	315	
2	C	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
4	E	99	3% 79% 15% 5%
5	F	443	10% 66% 12% 22%
6	G	21	10% 38% 38% 24%
7	H	27	7% 44% 41% 15%
8	I	3	33% 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28636 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1787	1141	311	333	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8761	5541	1562	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total	C	N	O	S	0	1	0
			11706	7425	2060	2186	35			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			326	154	62	94	16			

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	23	Total	C	N	O	P	0	0	0
			476	227	91	136	22			

- Molecule 8 is a RNA chain called RNA (5'-D(*PP*PP*P)-R(*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			75	29	12	29	5			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

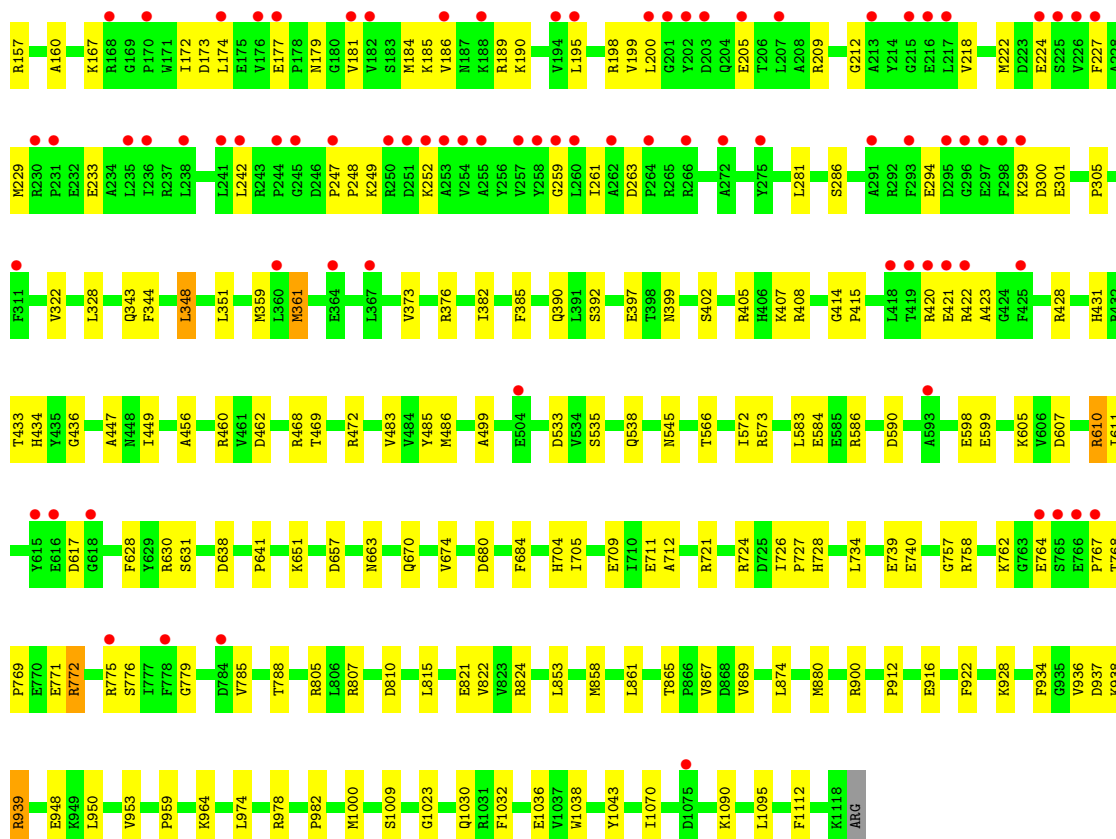
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Mg 1	0	0
9	D	3	Total 3	Mg 3	0	0
9	F	2	Total 2	Mg 2	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

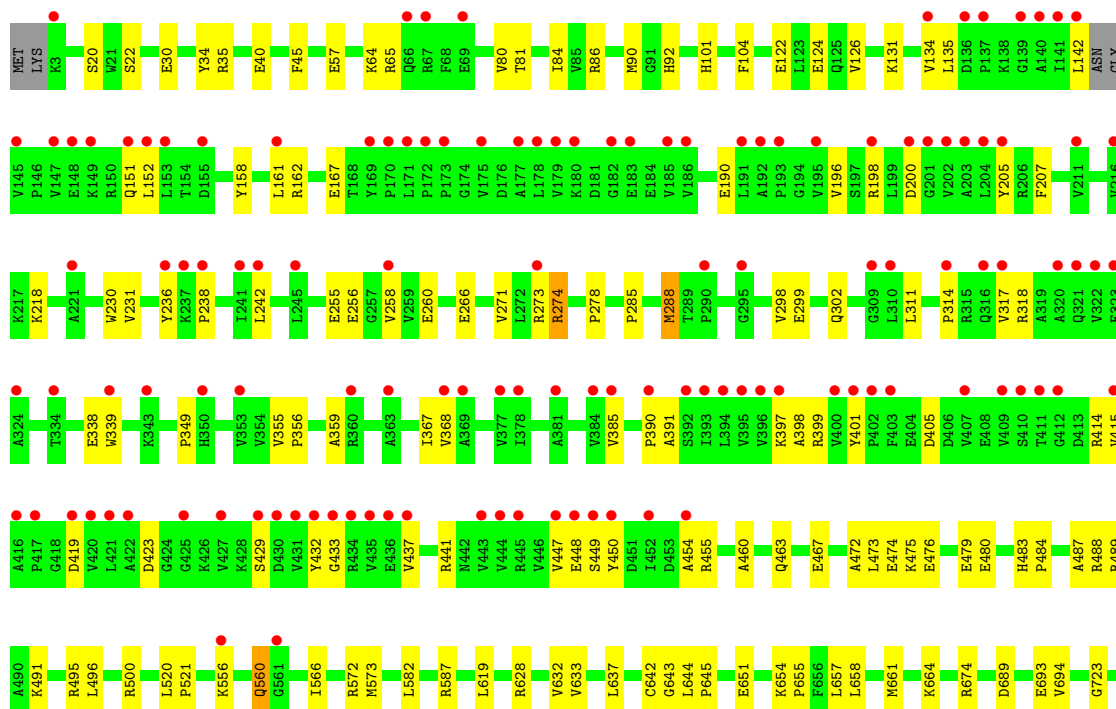
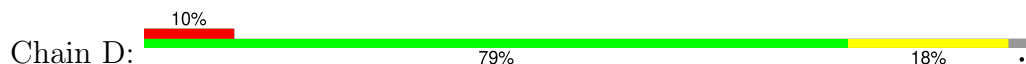
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total 2	Zn 2	0	0

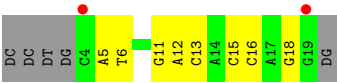
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	3	Total 3	O 3	0	0
11	B	4	Total 4	O 4	0	0
11	C	47	Total 47	O 47	0	0
11	D	72	Total 72	O 72	0	0
11	E	2	Total 2	O 2	0	0
11	F	6	Total 6	O 6	0	0
11	G	5	Total 5	O 5	0	0
11	I	1	Total 1	O 1	0	0

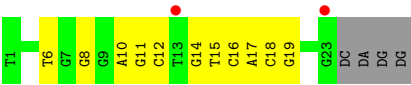


• Molecule 3: DNA-directed RNA polymerase subunit beta'





● Molecule 7: DNA (27-MER)



● Molecule 8: RNA (5'-D(*PP*PP*P)-R(*GP*GP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.42Å 103.70Å 295.44Å 90.00° 98.67° 90.00°	Depositor
Resolution (Å)	48.86 – 2.69 48.86 – 2.69	Depositor EDS
% Data completeness (in resolution range)	74.9 (48.86-2.69) 74.9 (48.86-2.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.212 , 0.260 0.213 , 0.256	Depositor DCC
R_{free} test set	2002 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28636	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, ZN

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	0/1819	0.35	0/2473
1	B	0.13	0/1821	0.34	0/2476
2	C	0.14	0/8927	0.36	0/12074
3	D	0.16	0/11914	0.35	0/16111
4	E	0.13	0/775	0.31	0/1045
5	F	0.14	0/2852	0.31	0/3837
6	G	0.18	0/365	0.38	0/560
7	H	0.22	0/535	0.43	0/826
8	I	0.12	0/47	0.26	0/71
All	All	0.15	0/29055	0.35	0/39473

There are no bond length outliers.

There are no bond angle outliers.

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	1787	0	1839	29	0
1	B	1789	0	1841	33	0
2	C	8761	0	8859	135	0
3	D	11706	0	11929	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	761	0	778	11	0
5	F	2807	0	2882	33	0
6	G	326	0	179	8	0
7	H	476	0	261	8	0
8	I	75	0	33	0	0
9	B	1	0	0	0	0
9	D	3	0	0	0	0
9	F	2	0	0	0	0
10	D	2	0	0	0	0
11	A	3	0	0	0	0
11	B	4	0	0	0	0
11	C	47	0	0	1	0
11	D	72	0	0	0	0
11	E	2	0	0	0	0
11	F	6	0	0	0	0
11	G	5	0	0	0	0
11	I	1	0	0	0	0
All	All	28636	0	28601	383	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 7.

All (383) 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:G:11:DG:H2'	6:G:12:DA:C8	2.20	0.76
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.68	0.74
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.69	0.72
3:D:65:ARG:NH1	5:F:378:GLY:O	2.21	0.72
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.70	0.72
7:H:14:DG:H2'	7:H:15:DT:H71	1.72	0.71
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.73	0.70
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.73	0.70
2:C:134:ARG:NH1	2:C:392:SER:O	2.25	0.70
3:D:256:GLU:O	3:D:274:ARG:NH1	2.26	0.69
2:C:198:ARG:HE	2:C:227:PHE:HA	1.57	0.67
3:D:162:ARG:O	3:D:414:ARG:NH1	2.28	0.67
6:G:12:DA:H2'	6:G:13:DC:C6	2.29	0.67
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.77	0.67
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.77	0.67
6:G:15:DC:H2'	6:G:16:DC:H6	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:190:GLU:HG2	3:D:196:VAL:HG22	1.77	0.66
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.77	0.66
3:D:1106:VAL:HG13	3:D:1220:ALA:H	1.61	0.66
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.78	0.66
2:C:776:SER:OG	5:F:373:LYS:NZ	2.29	0.65
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.77	0.65
3:D:657:LEU:HG	3:D:661:MET:HE2	1.78	0.65
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.78	0.65
5:F:370:LYS:HB3	5:F:376:ILE:HG12	1.78	0.65
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.78	0.64
1:B:91:ASN:ND2	1:B:93:SER:OG	2.30	0.64
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.80	0.64
6:G:15:DC:H2'	6:G:16:DC:C6	2.32	0.63
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.31	0.63
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.32	0.63
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.32	0.63
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.81	0.63
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.81	0.63
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.81	0.62
1:B:112:ARG:HG3	1:B:125:PRO:HB2	1.81	0.62
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.32	0.62
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.81	0.61
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.83	0.61
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.81	0.61
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.34	0.61
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.81	0.60
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.34	0.60
2:C:212:GLY:HA2	2:C:218:VAL:HG11	1.83	0.60
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.20	0.60
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.84	0.60
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.27	0.60
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.84	0.60
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.34	0.60
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.30	0.59
3:D:134:VAL:HG22	3:D:151:GLN:H	1.66	0.59
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.84	0.59
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.84	0.59
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.82	0.59
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.85	0.59
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.82	0.59
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:NH2	1:A:187:GLY:O	2.35	0.59
2:C:399:ASN:O	2:C:402:SER:OG	2.20	0.59
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.84	0.58
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.30	0.58
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.85	0.58
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.28	0.58
2:C:605:LYS:HB3	2:C:610:ARG:NH2	2.19	0.58
3:D:405:ASP:HB3	3:D:423:ASP:HA	1.84	0.58
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.36	0.57
2:C:468:ARG:NH2	11:C:1201:HOH:O	2.36	0.57
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.87	0.57
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.87	0.57
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.39	0.57
2:C:154:ARG:HE	2:C:157:ARG:HG3	1.69	0.56
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.87	0.56
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.87	0.56
3:D:968:ASP:O	3:D:971:LEU:HB2	2.06	0.56
7:H:18:DC:H2"	7:H:19:DG:C8	2.41	0.56
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.87	0.56
2:C:408:ARG:NH1	2:C:456:ALA:O	2.38	0.56
2:C:724:ARG:NH2	2:C:734:LEU:O	2.39	0.56
5:F:163:LEU:HB3	5:F:174:LEU:HD22	1.88	0.55
2:C:771:GLU:O	2:C:775:ARG:HG2	2.07	0.55
2:C:428:ARG:NH2	2:C:447:ALA:O	2.36	0.55
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.87	0.55
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.36	0.54
3:D:142:LEU:HD13	3:D:161:LEU:HD11	1.89	0.54
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.37	0.54
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.89	0.54
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.27	0.54
2:C:423:ALA:O	2:C:428:ARG:NH1	2.41	0.54
3:D:959:GLU:N	3:D:959:GLU:OE1	2.40	0.54
4:E:50:THR:HG22	4:E:51:LEU:H	1.73	0.54
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.90	0.54
1:B:220:GLU:O	1:B:223:THR:OG1	2.23	0.54
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.08	0.54
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.89	0.53
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.09	0.53
2:C:607:ASP:HB2	2:C:610:ARG:CZ	2.39	0.53
1:A:133:GLU:OE1	2:C:610:ARG:NH2	2.40	0.53
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.42	0.53
2:C:1009:SER:HB3	3:D:651:GLU:O	2.09	0.52
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.91	0.52
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.91	0.52
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.90	0.52
3:D:886:VAL:HB	3:D:900:ILE:HD11	1.91	0.52
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.92	0.52
3:D:843:PHE:HE2	3:D:864:VAL:HG11	1.75	0.52
2:C:118:ILE:HD11	2:C:344:PHE:CE1	2.45	0.52
3:D:260:GLU:HB3	3:D:271:VAL:HB	1.91	0.52
3:D:864:VAL:HG12	3:D:865:THR:H	1.75	0.52
3:D:828:LYS:HG2	3:D:833:GLU:HG2	1.92	0.52
3:D:433:GLY:HA2	3:D:449:SER:H	1.75	0.51
3:D:131:LYS:HD2	3:D:152:LEU:HD23	1.93	0.51
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.93	0.51
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.93	0.51
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.45	0.51
2:C:224:GLU:CD	2:C:224:GLU:H	2.18	0.51
3:D:273:ARG:HG2	3:D:278:PRO:HA	1.92	0.51
3:D:472:ALA:O	3:D:476:GLU:HG2	2.10	0.51
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.45	0.51
2:C:805:ARG:HH21	2:C:807:ARG:HD3	1.75	0.51
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.45	0.51
3:D:968:ASP:HA	3:D:971:LEU:HD12	1.92	0.51
2:C:184:MET:HE2	2:C:186:VAL:HG21	1.93	0.51
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.46	0.51
2:C:101:ILE:HG12	2:C:108:ILE:HG12	1.93	0.51
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.93	0.50
1:A:4:SER:O	1:A:189:ARG:NH2	2.44	0.50
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.12	0.50
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.47	0.50
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.93	0.50
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.94	0.50
2:C:628:PHE:H	2:C:638:ASP:CB	2.24	0.50
3:D:573:MET:SD	5:F:210:LEU:HB3	2.50	0.50
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.92	0.50
3:D:658:LEU:HD11	3:D:674[A]:ARG:HH11	1.76	0.50
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.46	0.50
1:A:110:LYS:HD3	1:A:128:HIS:HA	1.94	0.50
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.93	0.50
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.93	0.50
1:B:23:PHE:HB2	1:B:197:LEU:HB2	1.93	0.50
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.93	0.50
3:D:349:PRO:HB3	5:F:97:GLU:HG3	1.94	0.50
2:C:294:GLU:HB3	2:C:299:LYS:HE2	1.94	0.49
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.93	0.49
3:D:864:VAL:HG12	3:D:865:THR:N	2.28	0.49
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.94	0.49
3:D:285:PRO:HD2	3:D:288:MET:HE2	1.94	0.49
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.48	0.49
2:C:628:PHE:H	2:C:638:ASP:HB3	1.78	0.49
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.44	0.49
2:C:167:LYS:HG2	7:H:12:DC:H2'	1.93	0.49
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.46	0.49
2:C:286:SER:OG	2:C:301:GLU:OE2	2.24	0.49
2:C:937:ASP:OD1	2:C:938:LYS:N	2.46	0.49
1:B:58:ILE:HG12	1:B:140:MET:HE2	1.94	0.48
2:C:1:MET:HE3	2:C:900:ARG:HD2	1.95	0.48
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.95	0.48
2:C:436:GLY:HA2	2:C:538:GLN:O	2.13	0.48
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.95	0.48
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.48	0.48
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.93	0.48
2:C:772:ARG:H	2:C:772:ARG:HG2	1.49	0.48
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.79	0.48
2:C:584:GLU:OE2	2:C:584:GLU:N	2.44	0.48
3:D:658:LEU:HA	3:D:661:MET:HE3	1.96	0.48
2:C:545:ASN:HB3	2:C:583:LEU:HD23	1.96	0.48
3:D:974:ILE:HD13	3:D:991:GLN:HB3	1.96	0.48
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.28	0.47
2:C:861:LEU:HD12	2:C:865:THR:HB	1.97	0.47
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.95	0.47
6:G:5:DA:H2'	6:G:6:DT:H72	1.95	0.47
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.97	0.47
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.96	0.47
2:C:572:ILE:HG13	2:C:573:ARG:HG3	1.96	0.47
2:C:586:ARG:NH2	2:C:590:ASP:OD2	2.38	0.47
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.97	0.47
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.96	0.47
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.96	0.47
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.14	0.47
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.50	0.47
3:D:432:TYR:O	3:D:448:GLU:HA	2.15	0.47
4:E:37:ASN:OD1	4:E:37:ASN:N	2.41	0.47
1:B:89:PHE:HD2	1:B:146:ARG:HD2	1.80	0.47
2:C:376:ARG:HD3	5:F:276:ARG:HD2	1.97	0.47
3:D:255:GLU:OE1	3:D:274:ARG:NH2	2.40	0.47
3:D:1500:LYS:HB3	3:D:1500:LYS:HE2	1.57	0.47
1:A:229:GLN:HB2	1:B:11:PHE:O	2.14	0.46
2:C:173:ASP:O	2:C:184:MET:HA	2.14	0.46
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.96	0.46
7:H:16:DC:H2'	7:H:17:DA:C8	2.50	0.46
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.97	0.46
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.97	0.46
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.98	0.46
2:C:948:GLU:HG3	2:C:953:VAL:HG23	1.97	0.46
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.50	0.46
3:D:399:ARG:HB3	3:D:401:TYR:CE2	2.51	0.46
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.97	0.46
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.49	0.46
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	1.98	0.46
1:B:72:LYS:HG2	1:B:131:THR:OG1	2.15	0.46
2:C:195:LEU:O	2:C:199:VAL:HG23	2.16	0.46
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.97	0.46
3:D:1084:THR:O	3:D:1088:THR:HG23	2.16	0.46
3:D:1108:ARG:HD2	3:D:1198:TYR:O	2.16	0.46
7:H:8:DG:C8	7:H:8:DG:H5'	2.50	0.46
1:A:10:VAL:HG12	1:A:26:GLU:O	2.16	0.46
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.97	0.46
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.51	0.46
3:D:750:PRO:O	3:D:756:GLN:NE2	2.49	0.46
3:D:883:ALA:HA	3:D:900:ILE:HD13	1.97	0.46
2:C:431:HIS:HB3	2:C:434:HIS:CD2	2.51	0.46
2:C:607:ASP:HB2	2:C:610:ARG:NH2	2.31	0.46
2:C:769:PRO:HA	2:C:772:ARG:HG3	1.97	0.45
3:D:475:LYS:O	3:D:479:GLU:HG2	2.16	0.45
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.98	0.45
2:C:535:SER:O	2:C:538:GLN:HG2	2.16	0.45
3:D:1497:GLU:HA	3:D:1500:LYS:HB2	1.97	0.45
2:C:150:PRO:HG3	2:C:322:VAL:HG11	1.99	0.45
2:C:189:ARG:HD2	2:C:242:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1147:ARG:HH22	3:D:1369:GLU:CD	2.24	0.45
1:A:226:SER:O	1:A:228:PRO:HD3	2.16	0.45
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.47	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.17	0.45
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.97	0.45
2:C:402:SER:HA	2:C:566:THR:HG23	1.99	0.45
2:C:468:ARG:HA	2:C:486:MET:O	2.16	0.45
2:C:598:GLU:O	2:C:651:LYS:NZ	2.42	0.45
2:C:657:ASP:OD2	2:C:663:ASN:N	2.45	0.45
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	1.97	0.45
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.50	0.45
1:A:70:GLY:N	2:C:607:ASP:OD1	2.46	0.45
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.50	0.45
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.82	0.45
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.99	0.45
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.99	0.45
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.52	0.45
3:D:758:GLU:OE1	3:D:1476:THR:OG1	2.32	0.45
3:D:1296:SER:OG	3:D:1297:GLU:N	2.49	0.45
2:C:1030:GLN:OE1	3:D:628:ARG:NH1	2.42	0.45
3:D:45:PHE:O	3:D:86:ARG:NH2	2.50	0.45
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.98	0.45
3:D:122:GLU:O	3:D:126:VAL:HG23	2.16	0.45
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.98	0.45
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.99	0.44
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.98	0.44
5:F:369:LEU:HD21	5:F:405:LEU:HD12	1.99	0.44
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.99	0.44
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.98	0.44
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.50	0.44
2:C:172:ILE:HD13	2:C:184:MET:HE3	1.99	0.44
2:C:281:LEU:HD13	2:C:305:PRO:HB2	2.00	0.44
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.33	0.44
1:B:32:PHE:HA	1:B:35:THR:HB	1.99	0.44
1:B:72:LYS:HG3	1:B:73:GLU:N	2.31	0.44
2:C:205:GLU:O	2:C:209:ARG:HG2	2.18	0.44
2:C:390:GLN:HB3	2:C:414:GLY:HA2	2.00	0.44
5:F:160:ASP:O	5:F:164:LYS:HD3	2.18	0.44
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.53	0.44
1:B:110:LYS:HD3	1:B:128:HIS:HA	2.00	0.44
2:C:880:MET:HG2	3:D:1038:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:135:LEU:HD23	3:D:463:GLN:HG2	2.00	0.44
3:D:1267:ARG:NE	3:D:1331:ASP:OD2	2.51	0.44
3:D:463:GLN:O	3:D:467:GLU:HG2	2.17	0.44
7:H:16:DC:H2''	7:H:17:DA:H5'	1.99	0.44
3:D:256:GLU:HG2	3:D:299:GLU:HA	1.99	0.44
5:F:362:SER:OG	5:F:365:GLU:HG2	2.18	0.44
2:C:726:ILE:HD11	2:C:757:GLY:HA3	2.00	0.44
5:F:84:TYR:O	5:F:88:ILE:HG12	2.17	0.44
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.77	0.43
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.53	0.43
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.18	0.43
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.51	0.43
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.98	0.43
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.00	0.43
2:C:179:ASN:HD21	2:C:181:VAL:HG12	1.83	0.43
2:C:431:HIS:HB3	2:C:434:HIS:HD2	1.82	0.43
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.00	0.43
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.53	0.43
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.00	0.43
3:D:398:ALA:HB2	3:D:447:VAL:HG22	2.00	0.43
2:C:874:LEU:O	3:D:1029:ARG:HG3	2.18	0.43
5:F:109:GLY:O	5:F:113:ILE:HG13	2.18	0.43
5:F:181:GLU:O	5:F:185:GLN:HG2	2.19	0.43
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.00	0.43
2:C:361:MET:HE3	2:C:361:MET:HB3	1.80	0.43
4:E:57:ASP:O	4:E:63:TRP:NE1	2.46	0.43
1:A:228:PRO:HB3	1:B:13:VAL:HG21	2.01	0.43
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.00	0.43
2:C:328:LEU:HD12	2:C:433:THR:O	2.18	0.43
3:D:207:PHE:HD2	3:D:391:ALA:HB3	1.84	0.43
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.54	0.43
2:C:259:GLY:HA2	2:C:263:ASP:HB2	2.01	0.43
2:C:853:LEU:HB2	2:C:858:MET:CE	2.45	0.43
2:C:1023:GLY:HA2	6:G:18:DG:OP2	2.19	0.43
3:D:314:PRO:HB2	3:D:317:VAL:HG12	2.00	0.43
2:C:20:GLU:O	2:C:24:GLU:HB2	2.18	0.43
3:D:654:LYS:O	3:D:658:LEU:HG	2.18	0.43
3:D:1147:ARG:HD3	3:D:1188:VAL:HG21	2.01	0.43
3:D:1441:GLN:HG2	6:G:12:DA:H5''	2.01	0.43
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.54	0.42
2:C:772:ARG:NE	5:F:380:GLU:OE2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.82	0.42
1:B:56:VAL:HG22	1:B:142:VAL:HG12	2.01	0.42
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.53	0.42
3:D:255:GLU:HB3	3:D:274:ARG:HH12	1.84	0.42
3:D:258:VAL:HG12	3:D:273:ARG:O	2.19	0.42
3:D:419:ASP:H	3:D:429:SER:HB3	1.84	0.42
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.00	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.89	0.42
2:C:348:LEU:HD12	2:C:348:LEU:HA	1.87	0.42
3:D:572:ARG:NH1	5:F:83:GLN:HB3	2.34	0.42
2:C:805:ARG:HE	2:C:807:ARG:HD3	1.85	0.42
1:B:85:LEU:HG	1:B:87:VAL:HG23	2.02	0.42
2:C:121:MET:SD	2:C:125:GLY:HA2	2.60	0.42
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.00	0.42
2:C:218:VAL:HG22	2:C:222:MET:HE2	2.00	0.42
3:D:230:TRP:CD1	3:D:231:VAL:H	2.38	0.42
4:E:44:GLU:OE2	4:E:72:ARG:NH1	2.41	0.42
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.93	0.42
3:D:556:LYS:O	3:D:560:GLN:HG3	2.19	0.42
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	2.01	0.42
2:C:858:MET:HG2	2:C:867:VAL:O	2.19	0.42
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.35	0.42
3:D:1341:PRO:HB3	3:D:1376:MET:HE2	2.00	0.42
3:D:1499:ARG:C	3:D:1501:GLU:H	2.27	0.42
2:C:611:ILE:HD11	2:C:641:PRO:HB3	2.02	0.41
2:C:767:PRO:HB2	2:C:772:ARG:HD2	2.03	0.41
3:D:637:LEU:O	3:D:935:LYS:NZ	2.53	0.41
2:C:91:GLN:HB2	2:C:117:HIS:HB3	2.01	0.41
2:C:420:ARG:C	2:C:422:ARG:H	2.28	0.41
3:D:689:ASP:CG	4:E:51:LEU:HD11	2.45	0.41
5:F:88:ILE:HG22	5:F:193:ARG:HG2	2.02	0.41
5:F:321:ILE:O	5:F:327:SER:HB3	2.19	0.41
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.95	0.41
2:C:928:LYS:HE3	2:C:928:LYS:HB2	1.68	0.41
3:D:1168:MET:HE3	3:D:1168:MET:HA	2.01	0.41
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.95	0.41
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.01	0.41
2:C:420:ARG:O	2:C:421:GLU:HB3	2.21	0.41
2:C:939:ARG:HG2	2:C:982:PRO:HD3	2.03	0.41
5:F:93:LEU:HD11	7:H:6:DT:H2"	2.01	0.41
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:HB2	1:A:20:TYR:HB3	2.02	0.41
1:A:184:THR:O	1:A:192:LEU:HB2	2.20	0.41
2:C:177:GLU:OE1	2:C:179:ASN:ND2	2.54	0.41
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.85	0.41
2:C:758:ARG:HH21	2:C:788:THR:HB	1.85	0.41
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.21	0.41
1:B:128:HIS:HE1	1:B:131:THR:HG22	1.86	0.41
3:D:924:MET:HE2	3:D:924:MET:HB3	1.91	0.41
7:H:10:DA:H2''	7:H:11:DG:C8	2.55	0.41
1:A:227:ASN:HD21	1:A:229:GLN:HE22	1.67	0.41
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.56	0.41
2:C:56:GLU:C	2:C:359:MET:HE3	2.46	0.41
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.02	0.41
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.20	0.41
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.91	0.41
4:E:33:HIS:NE2	4:E:89:MET:HB3	2.35	0.41
2:C:249:LYS:HB3	2:C:252:LYS:HB2	2.02	0.41
3:D:841:TYR:HB2	3:D:864:VAL:HG13	2.02	0.41
3:D:1053:PHE:CE2	3:D:1072:ILE:HG23	2.55	0.41
3:D:1232:PRO:HG2	3:D:1356:TYR:HE1	1.86	0.41
5:F:102:LEU:O	5:F:106:VAL:HG23	2.21	0.41
6:G:11:DG:H2'	6:G:12:DA:H8	1.78	0.41
2:C:118:ILE:HG12	2:C:382:ILE:HD13	2.03	0.40
3:D:90:MET:HE3	3:D:90:MET:HB3	1.96	0.40
3:D:645:PRO:HB3	3:D:723:GLY:O	2.21	0.40
1:A:112:ARG:NH1	1:A:126:ASP:OD1	2.48	0.40
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.03	0.40
1:B:124:ASN:OD1	1:B:124:ASN:N	2.54	0.40
2:C:712:ALA:HB3	2:C:821:GLU:HG3	2.03	0.40
3:D:134:VAL:CG2	3:D:151:GLN:H	2.32	0.40
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.56	0.40
3:D:879:ARG:HD3	3:D:902:LEU:O	2.21	0.40
3:D:1432:LYS:HE3	3:D:1432:LYS:HB2	1.85	0.40
2:C:727:PRO:HB2	2:C:728:HIS:ND1	2.37	0.40
3:D:200:ASP:O	3:D:397:LYS:HG2	2.22	0.40
2:C:775:ARG:O	2:C:779:GLY:N	2.53	0.40
2:C:912:PRO:O	2:C:916:GLU:HG3	2.22	0.40
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.56	0.40
3:D:1211:MET:HE1	4:E:16:LYS:HD2	2.04	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	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	221 (98%)	4 (2%)	0	100	100
2	C	1108/1119 (99%)	1078 (97%)	30 (3%)	0	100	100
3	D	1479/1524 (97%)	1448 (98%)	31 (2%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	341 (99%)	3 (1%)	0	100	100
All	All	3473/3815 (91%)	3400 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	199/273 (73%)	194 (98%)	5 (2%)	42	71
1	B	200/273 (73%)	196 (98%)	4 (2%)	48	76
2	C	934/941 (99%)	914 (98%)	20 (2%)	47	75
3	D	1247/1279 (98%)	1222 (98%)	25 (2%)	48	76
4	E	83/88 (94%)	81 (98%)	2 (2%)	43	72
5	F	301/388 (78%)	293 (97%)	8 (3%)	39	69
All	All	2964/3242 (91%)	2900 (98%)	64 (2%)	45	74

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	134	GLU
1	A	142	VAL
1	A	205	VAL
1	A	229	GLN
1	B	10	VAL
1	B	133	GLU
1	B	154	GLU
1	B	227	ASN
2	C	1	MET
2	C	100	LEU
2	C	138	SER
2	C	190	LYS
2	C	261	ILE
2	C	348	LEU
2	C	361	MET
2	C	405	ARG
2	C	449	ILE
2	C	599	GLU
2	C	610	ARG
2	C	617	ASP
2	C	670	GLN
2	C	739	GLU
2	C	762	LYS
2	C	764	GLU
2	C	772	ARG
2	C	815	LEU
2	C	939	ARG
2	C	950	LEU
3	D	20	SER
3	D	80	VAL
3	D	81	THR
3	D	84	ILE
3	D	274	ARG
3	D	288	MET
3	D	450	TYR
3	D	560	GLN
3	D	632	VAL
3	D	694	VAL
3	D	754	PHE
3	D	783	ARG
3	D	784	ASP

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Mol	Chain	Res	Type
3	D	810	GLU
3	D	907	GLU
3	D	1128	VAL
3	D	1154	GLU
3	D	1221	VAL
3	D	1305	LEU
3	D	1366	LYS
3	D	1408	ILE
3	D	1418	LYS
3	D	1433	SER
3	D	1488	ASP
3	D	1500	LYS
4	E	50	THR
4	E	74	VAL
5	F	110	MET
5	F	141	VAL
5	F	155	THR
5	F	156	VAL
5	F	279	GLN
5	F	295	MET
5	F	324	GLU
5	F	346	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	188	GLN
1	A	227	ASN
1	B	91	ASN
1	B	188	GLN
1	B	212	ASN
2	C	117	HIS
2	C	187	ASN
2	C	538	GLN
2	C	567	GLN
2	C	1047	HIS
2	C	1064	ASN
3	D	442	ASN
3	D	696	HIS
3	D	737	ASN
3	D	1195	GLN

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Mol	Chain	Res	Type
3	D	1442	ASN
3	D	1489	GLN
5	F	83	GLN
5	F	269	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/3 (33%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/315 (72%)	0.21	1 (0%) 88 87	26, 41, 65, 77	0
1	B	227/315 (72%)	0.60	11 (4%) 35 32	25, 52, 80, 109	0
2	C	1112/1119 (99%)	0.18	87 (7%) 19 16	7, 36, 97, 122	0
3	D	1484/1524 (97%)	0.38	160 (10%) 11 9	8, 38, 96, 123	1 (0%)
4	E	94/99 (94%)	0.09	3 (3%) 50 46	17, 38, 73, 83	0
5	F	346/443 (78%)	0.76	45 (13%) 7 6	17, 55, 91, 111	0
6	G	16/21 (76%)	0.60	2 (12%) 8 7	29, 49, 123, 131	0
7	H	23/27 (85%)	0.99	2 (8%) 16 13	52, 72, 120, 136	0
8	I	2/3 (66%)	2.47	1 (50%) 0 0	23, 23, 23, 38	2 (100%)
All	All	3531/3866 (91%)	0.35	312 (8%) 15 13	7, 41, 95, 136	3 (0%)

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	203	ALA	6.0
3	D	420	VAL	5.6
3	D	142	LEU	5.5
2	C	275	TYR	5.1
3	D	1252	ILE	4.8
2	C	188	LYS	4.7
3	D	1283	ILE	4.4
3	D	141	ILE	4.4
3	D	434	ARG	4.3
3	D	415	VAL	4.3
3	D	1128	VAL	4.3
1	B	6	LEU	4.3
2	C	419	THR	4.2
3	D	170	PRO	4.1
8	I	8	U	4.1

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Mol	Chain	Res	Type	RSRZ
3	D	447	VAL	4.1
3	D	409	VAL	4.0
3	D	182	GLY	4.0
5	F	138	SER	3.9
2	C	766	GLU	3.9
3	D	1129	THR	3.8
3	D	369	ALA	3.8
2	C	236	ILE	3.8
3	D	242	LEU	3.8
3	D	322	VAL	3.8
5	F	139	ALA	3.7
3	D	161	LEU	3.7
3	D	236	TYR	3.7
3	D	202	VAL	3.7
2	C	254	VAL	3.6
3	D	186	VAL	3.6
3	D	452	ILE	3.6
5	F	78	SER	3.6
3	D	295	GLY	3.5
3	D	416	ALA	3.5
3	D	183	GLU	3.5
3	D	368	VAL	3.5
3	D	1130	ARG	3.5
2	C	297	GLU	3.4
2	C	298	PHE	3.4
3	D	443	VAL	3.4
3	D	1281	VAL	3.4
3	D	1294	VAL	3.4
3	D	1313	VAL	3.4
3	D	400	VAL	3.4
5	F	323	ASP	3.4
3	D	145	VAL	3.3
3	D	396	VAL	3.3
3	D	205	TYR	3.3
2	C	207	LEU	3.3
3	D	1499	ARG	3.3
2	C	311	PHE	3.3
2	C	177	GLU	3.3
3	D	433	GLY	3.3
5	F	146	GLY	3.3
5	F	148	LYS	3.3
3	D	195	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	193	PRO	3.2
3	D	401	TYR	3.2
3	D	393	ILE	3.2
2	C	231	PRO	3.2
3	D	180	LYS	3.2
3	D	449	SER	3.2
3	D	432	TYR	3.2
2	C	242	LEU	3.2
5	F	170	HIS	3.2
3	D	1502	ALA	3.2
5	F	144	ILE	3.2
1	B	67	THR	3.2
3	D	201	GLY	3.2
3	D	412	GLY	3.2
2	C	425	PHE	3.1
3	D	435	VAL	3.1
3	D	1299	PHE	3.1
2	C	299	LYS	3.1
3	D	454	ALA	3.1
2	C	264	PRO	3.0
3	D	173	PRO	3.0
3	D	437	VAL	3.0
3	D	152	LEU	3.0
1	B	7	LYS	3.0
5	F	414	ARG	3.0
2	C	259	GLY	3.0
4	E	95	VAL	3.0
5	F	147	LEU	3.0
3	D	140	ALA	3.0
2	C	293	PHE	3.0
2	C	103	LYS	2.9
3	D	177	ALA	2.9
2	C	266	ARG	2.9
5	F	135	ILE	2.9
5	F	137	GLY	2.9
3	D	178	LEU	2.9
2	C	215	GLY	2.9
2	C	255	ALA	2.9
2	C	767	PRO	2.8
3	D	410	SER	2.8
3	D	191	LEU	2.8
3	D	429	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	295	ASP	2.8
3	D	1498	ALA	2.8
5	F	104	ARG	2.8
5	F	149	GLU	2.8
3	D	172	PRO	2.8
1	A	4	SER	2.8
3	D	972	LEU	2.8
3	D	427	VAL	2.8
3	D	445	ARG	2.8
7	H	23	DG	2.7
5	F	136	LEU	2.7
2	C	364	GLU	2.7
2	C	253	ALA	2.7
3	D	258	VAL	2.7
2	C	244	PRO	2.7
3	D	343	LYS	2.7
3	D	402	PRO	2.7
3	D	169	TYR	2.7
2	C	107	LEU	2.7
3	D	436	GLU	2.7
2	C	213	ALA	2.7
3	D	147	VAL	2.7
3	D	324	ALA	2.7
3	D	407	VAL	2.7
3	D	1314	LYS	2.7
3	D	390	PRO	2.7
5	F	142	ARG	2.6
3	D	556	LYS	2.6
2	C	593	ALA	2.6
3	D	316	GLN	2.6
3	D	430	ASP	2.6
1	B	100	LEU	2.6
3	D	153	LEU	2.6
3	D	561	GLY	2.6
3	D	1286	THR	2.6
2	C	203	ASP	2.6
5	F	423	ASP	2.6
2	C	200	LEU	2.6
3	D	1500	LYS	2.6
2	C	56	GLU	2.6
3	D	69	GLU	2.6
2	C	291	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	137	PRO	2.6
5	F	415	THR	2.6
5	F	110	MET	2.6
5	F	422	LEU	2.6
2	C	422	ARG	2.6
2	C	176	VAL	2.6
3	D	431	VAL	2.6
5	F	153	PRO	2.6
3	D	321	GLN	2.6
3	D	1300	SER	2.5
3	D	204	LEU	2.5
3	D	237	LYS	2.5
2	C	182	VAL	2.5
3	D	317	VAL	2.5
3	D	363	ALA	2.5
3	D	422	ALA	2.5
5	F	393	THR	2.5
2	C	418	LEU	2.5
3	D	421	LEU	2.5
2	C	225	SER	2.5
3	D	241	ILE	2.5
2	C	201	GLY	2.5
1	B	5	LYS	2.5
3	D	1490	LYS	2.5
2	C	250	ARG	2.5
3	D	200	ASP	2.5
3	D	419	ASP	2.5
3	D	1497	GLU	2.5
2	C	63	GLY	2.5
3	D	211	VAL	2.5
3	D	1289	LYS	2.4
3	D	216	VAL	2.4
3	D	245	LEU	2.4
3	D	290	PRO	2.4
3	D	149	LYS	2.4
3	D	378	ILE	2.4
5	F	151	LEU	2.4
5	F	166	LEU	2.4
6	G	4	DC	2.4
3	D	1501	GLU	2.4
2	C	247	PRO	2.4
3	D	139	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	273	ARG	2.4
3	D	802	ALA	2.4
2	C	235	LEU	2.4
2	C	238	LEU	2.4
2	C	616	GLU	2.4
3	D	1127	GLU	2.4
3	D	339	TRP	2.4
3	D	66	GLN	2.4
5	F	399	GLN	2.4
2	C	226	VAL	2.4
5	F	141	VAL	2.4
2	C	217	LEU	2.3
6	G	19	DG	2.3
3	D	309	GLY	2.3
3	D	353	VAL	2.3
2	C	227	PHE	2.3
2	C	260	LEU	2.3
5	F	175	HIS	2.3
2	C	765	SER	2.3
3	D	360	ARG	2.3
2	C	257	VAL	2.3
3	D	444	VAL	2.3
2	C	195	LEU	2.3
2	C	262	ALA	2.3
3	D	221	ALA	2.3
3	D	1305	LEU	2.3
5	F	143	HIS	2.3
2	C	615	TYR	2.3
1	B	189	ARG	2.3
2	C	296	GLY	2.3
3	D	385	VAL	2.3
3	D	395	VAL	2.3
2	C	252	LYS	2.3
5	F	173	TYR	2.3
2	C	504	GLU	2.3
2	C	775	ARG	2.3
3	D	417	PRO	2.3
3	D	425	GLY	2.3
2	C	778	PHE	2.3
3	D	192	ALA	2.2
3	D	980	MET	2.2
3	D	148	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	230	ARG	2.2
2	C	618	GLY	2.2
3	D	179	VAL	2.2
3	D	185	VAL	2.2
3	D	310	LEU	2.2
3	D	377	VAL	2.2
2	C	272	ALA	2.2
3	D	448	GLU	2.2
5	F	111	GLU	2.2
5	F	120	THR	2.2
2	C	420	ARG	2.2
3	D	392	SER	2.2
4	E	53	GLY	2.2
4	E	51	LEU	2.2
3	D	3	LYS	2.2
5	F	113	ILE	2.2
3	D	320	ALA	2.2
2	C	205	GLU	2.2
2	C	764	GLU	2.2
3	D	323	GLU	2.2
2	C	245	GLY	2.2
2	C	367	LEU	2.2
5	F	88	ILE	2.2
3	D	807	ALA	2.2
3	D	411	THR	2.2
3	D	67	ARG	2.2
3	D	1318	TYR	2.2
7	H	13	DT	2.2
1	B	2	LEU	2.2
3	D	394	LEU	2.2
5	F	122	LEU	2.2
2	C	251	ASP	2.2
2	C	784	ASP	2.2
3	D	1315	ASP	2.2
3	D	134	VAL	2.2
3	D	175	VAL	2.2
3	D	974	ILE	2.2
3	D	403	PHE	2.2
5	F	133	ALA	2.1
2	C	216	GLU	2.1
2	C	224	GLU	2.1
3	D	1287	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	198	ARG	2.1
3	D	334	THR	2.1
2	C	170	PRO	2.1
2	C	202	TYR	2.1
2	C	421	GLU	2.1
2	C	149	THR	2.1
3	D	314	PRO	2.1
3	D	151	GLN	2.1
2	C	258	TYR	2.1
3	D	450	TYR	2.1
5	F	229	TYR	2.1
2	C	102	HIS	2.1
5	F	145	PRO	2.1
2	C	174	LEU	2.1
2	C	360	LEU	2.1
5	F	102	LEU	2.1
1	B	57	TYR	2.1
5	F	397	ILE	2.1
5	F	128	ARG	2.1
5	F	150	THR	2.1
1	B	62	LEU	2.1
2	C	241	LEU	2.1
5	F	174	LEU	2.1
2	C	181	VAL	2.1
3	D	384	VAL	2.1
5	F	389	PHE	2.1
2	C	168	ARG	2.0
2	C	1075	ASP	2.0
3	D	136	ASP	2.0
1	B	93	SER	2.0
3	D	1131	SER	2.0
3	D	397	LYS	2.0
3	D	238	PRO	2.0
5	F	119	ILE	2.0
2	C	186	VAL	2.0
2	C	194	VAL	2.0
2	C	104	ASP	2.0
3	D	155	ASP	2.0
3	D	381	ALA	2.0
5	F	403	LYS	2.0
3	D	1491	THR	2.0
3	D	171	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	350	HIS	2.0
1	B	58	ILE	2.0
3	D	870	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	B	401	1/1	0.81	0.11	60,60,60,60	0
9	MG	D	1605	1/1	0.86	0.09	41,41,41,41	0
9	MG	F	501	1/1	0.91	0.07	41,41,41,41	0
9	MG	F	502	1/1	0.91	0.22	43,43,43,43	0
9	MG	D	1604	1/1	0.92	0.20	33,33,33,33	0
9	MG	D	1603	1/1	0.99	0.05	18,18,18,18	0
10	ZN	D	1601	1/1	0.99	0.03	23,23,23,23	0
10	ZN	D	1602	1/1	1.00	0.01	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.